Math 692A: Geometric Numerical Integration

Melvin Leok

Mathematics, Purdue University.

mleok@math.purdue.edu
http://www.math.purdue.edu/~mleok/

PURDUE UNIVERSITY

Mathematics, Purdue University
NSF DMS-0504747, 0714223 and DMS-0726263

The Mathematics of Falling Cats

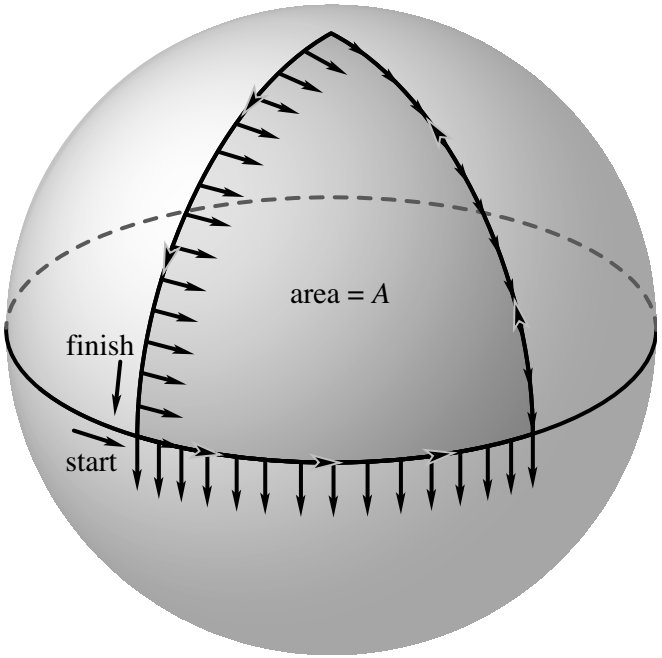
Connections, Curvature, and Geometric Phase

Connections

- **Connections** provide a means of comparing elements of a fiber based at different points on the manifold.

Holonomy and Curvature

- **Geometric Phase** is an example of **holonomy**.
- **Curvature** can be thought of as **infinitesimal holonomy**.



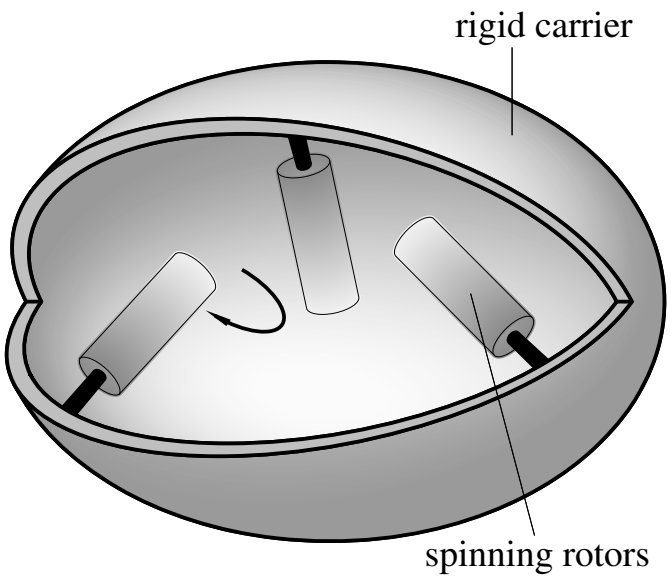
Example of Holonomy

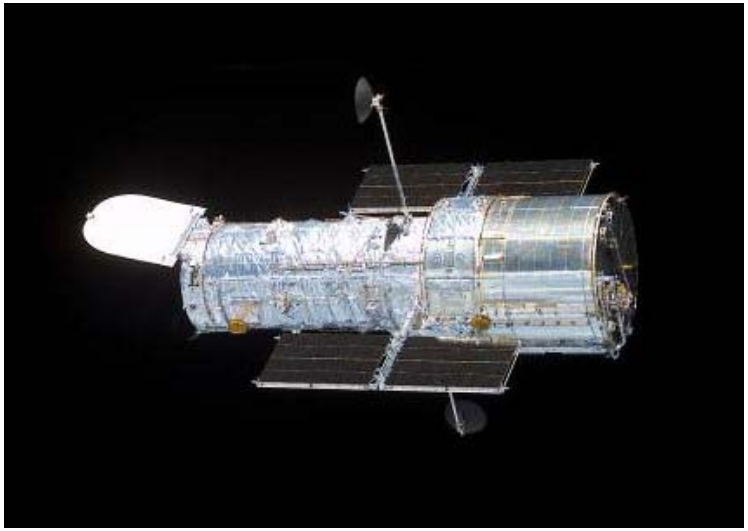
Vatican Museum double helical staircase designed by Giuseppe Momo in 1932.

Geometric Control of Spacecraft

Geometric Phase based controllers

- Shape controlled using internal momentum wheels and gyroscopes.
- Changes in shape result in corresponding changes in orientation.
- More precise than chemical propulsion based orientation control.



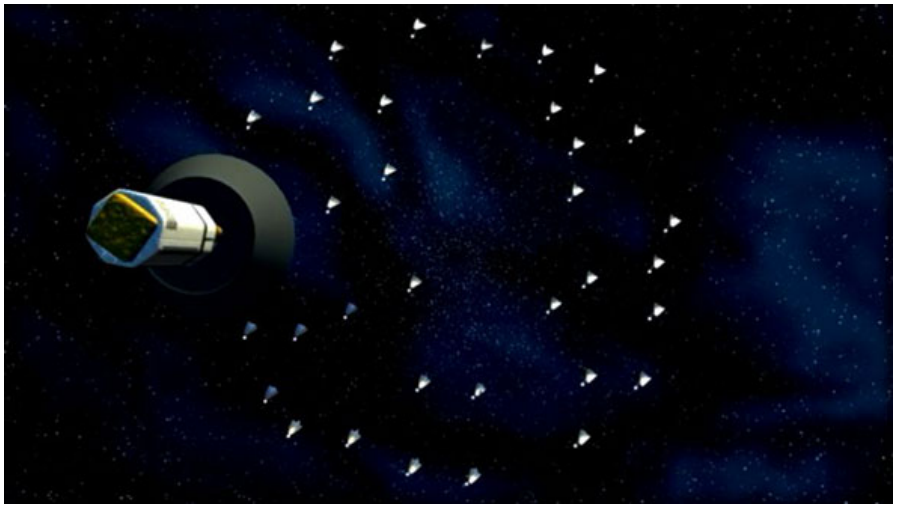


Geometric Control of Spacecraft

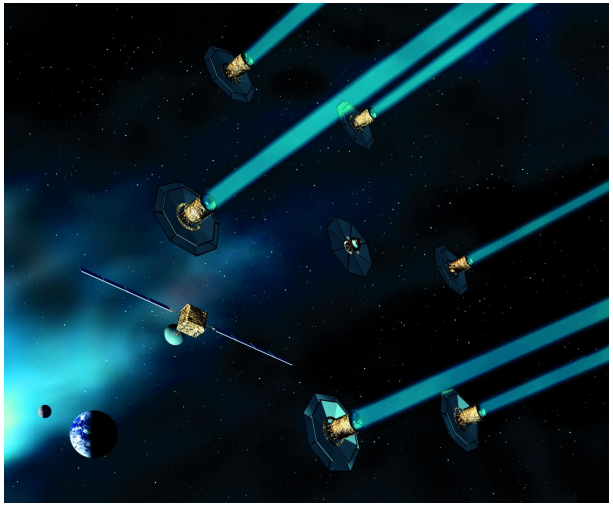
Shape Dynamics of Formations of Satellites

NASA Terrestrial Planet Finder (TPF)

- The NASA Terrestrial Planet Finder (TPF) and the ESA Darwin missions are examples of a potential application of the geometric formation control of satellite clusters.



Small satellites in arranged in a formation to yield a large effective aperture telescope. Courtesy NASA/JPL-Caltech.



Artist's conception of the ESA Darwin flotilla. Courtesy ESA.

- It is quite natural to think of controlling the shape of the cluster, and its orientation (group) separately.

Numerically implementing geometric control algorithms

Demand for long-time stability in control algorithms

- Trend towards autonomous space and underwater vehicle missions with **long deployment times** and **low energy propulsion systems**.
- Small inaccuracies in the control algorithms accumulated over long times will significantly diminish the operational lifespan of such missions.
- Need for geometric integrators to efficiently achieve good qualitative results for simulations over long times.

Geometry and Numerical Methods

Dynamical equations preserve structure

- Many continuous systems of interest have properties that are conserved by the flow:
  - Energy
  - Symmetries, Reversibility, Monotonicity
  - Momentum - Angular, Linear, Kelvin Circulation Theorem.
  - Symplectic Form
  - Integrability
- At other times, the equations themselves are defined on a manifold, such as a Lie group, or more general configuration manifold of a mechanical system, and the discrete trajectory we compute should remain on this manifold, since the equations may not be well-defined off the surface.

Motivation: Geometric Integration

Main Goal of Geometric Integration:

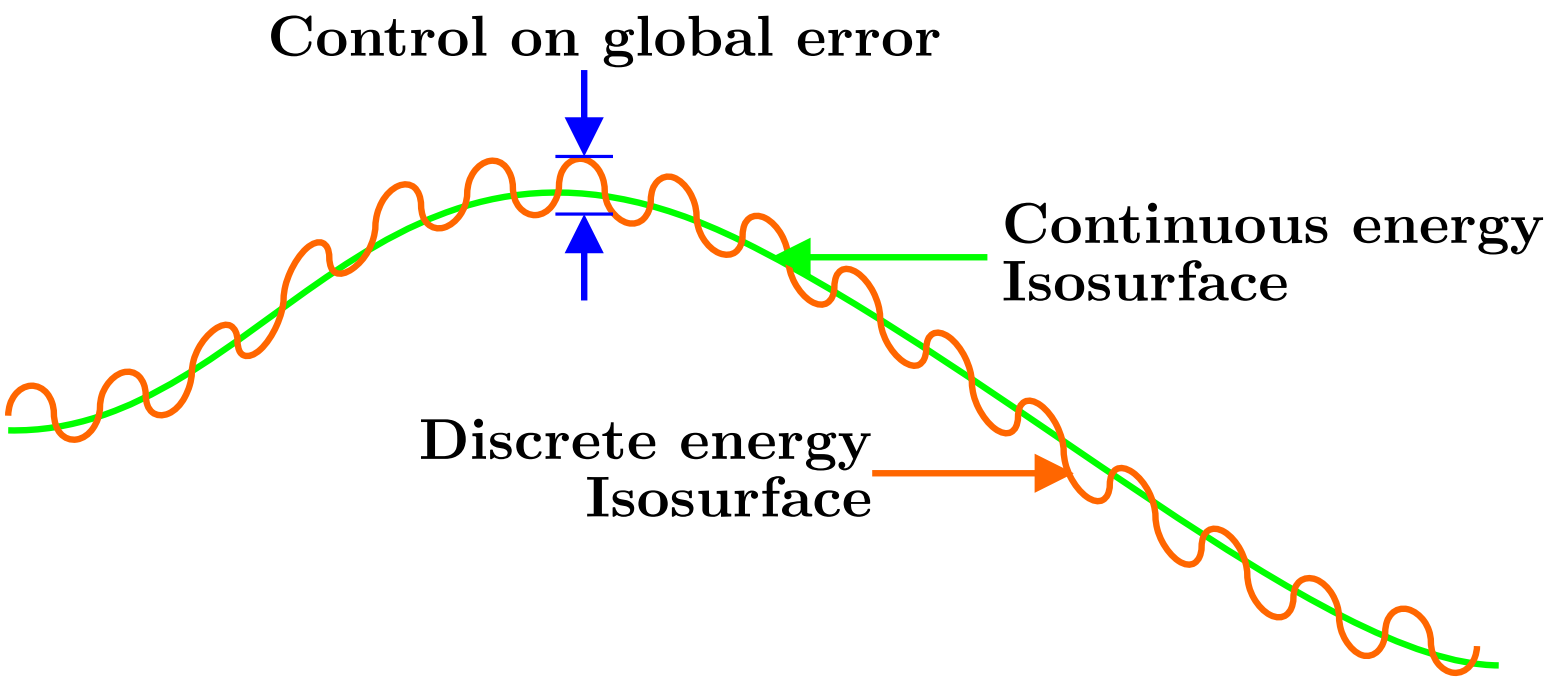
Structure preservation in order to reproduce long time behavior.

Role of Discrete Structure-Preservation:

Discrete conservation laws impart long time numerical stability to computations, since the structure-preserving algorithm exactly conserves a discrete quantity that is always close to the continuous quantity we are interested in.

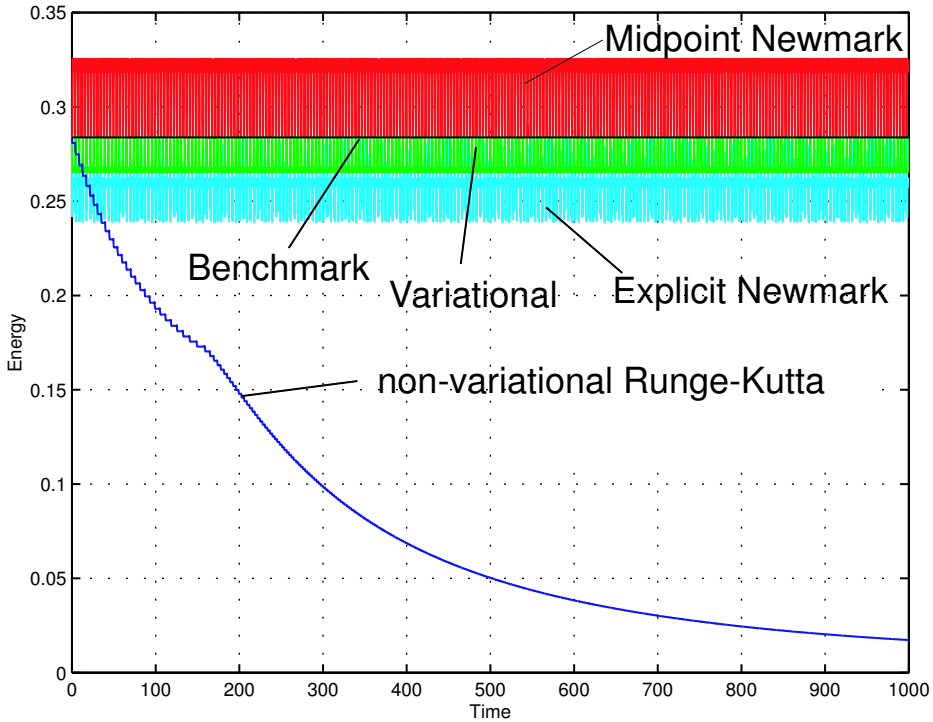
Geometric Integration: Energy Stability

- Energy stability for symplectic integrators

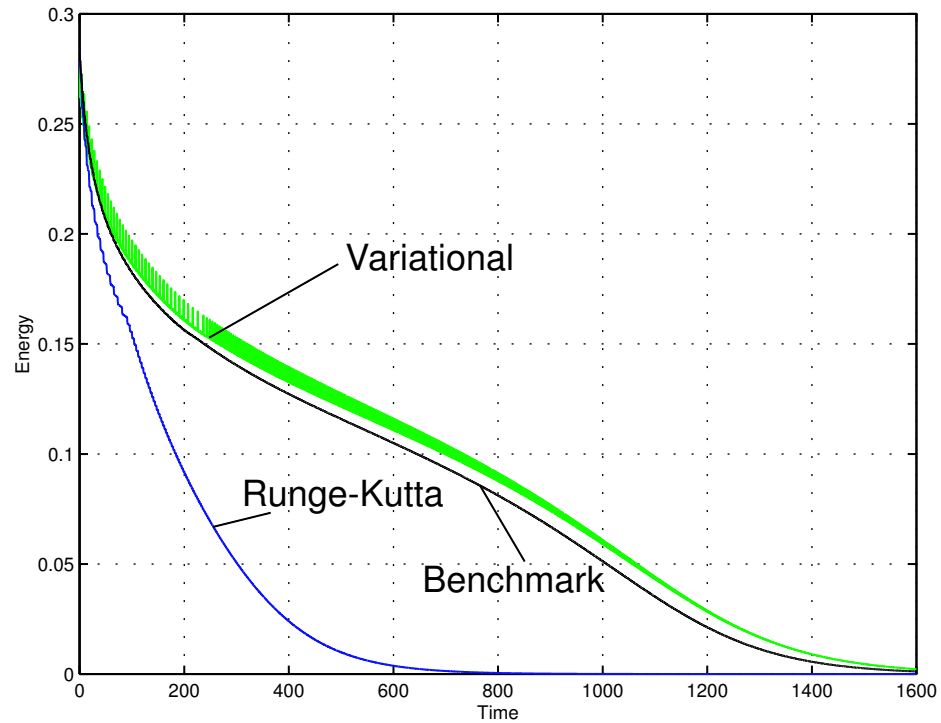


Geometric Integration: Energy Stability

- Energy behavior for conservative and dissipative systems



(a) Conservative mechanics



(b) Dissipative mechanics

Geometric Integration: Energy Stability

Solar System Simulation

- Forward Euler

$$\mathbf{q}_{k+1} = \mathbf{q}_k + h\dot{\mathbf{q}}(\mathbf{q}_k, \mathbf{p}_k),$$
$$\mathbf{p}_{k+1} = \mathbf{p}_k + h\dot{\mathbf{p}}(\mathbf{q}_k, \mathbf{p}_k).$$

- Inverse Euler

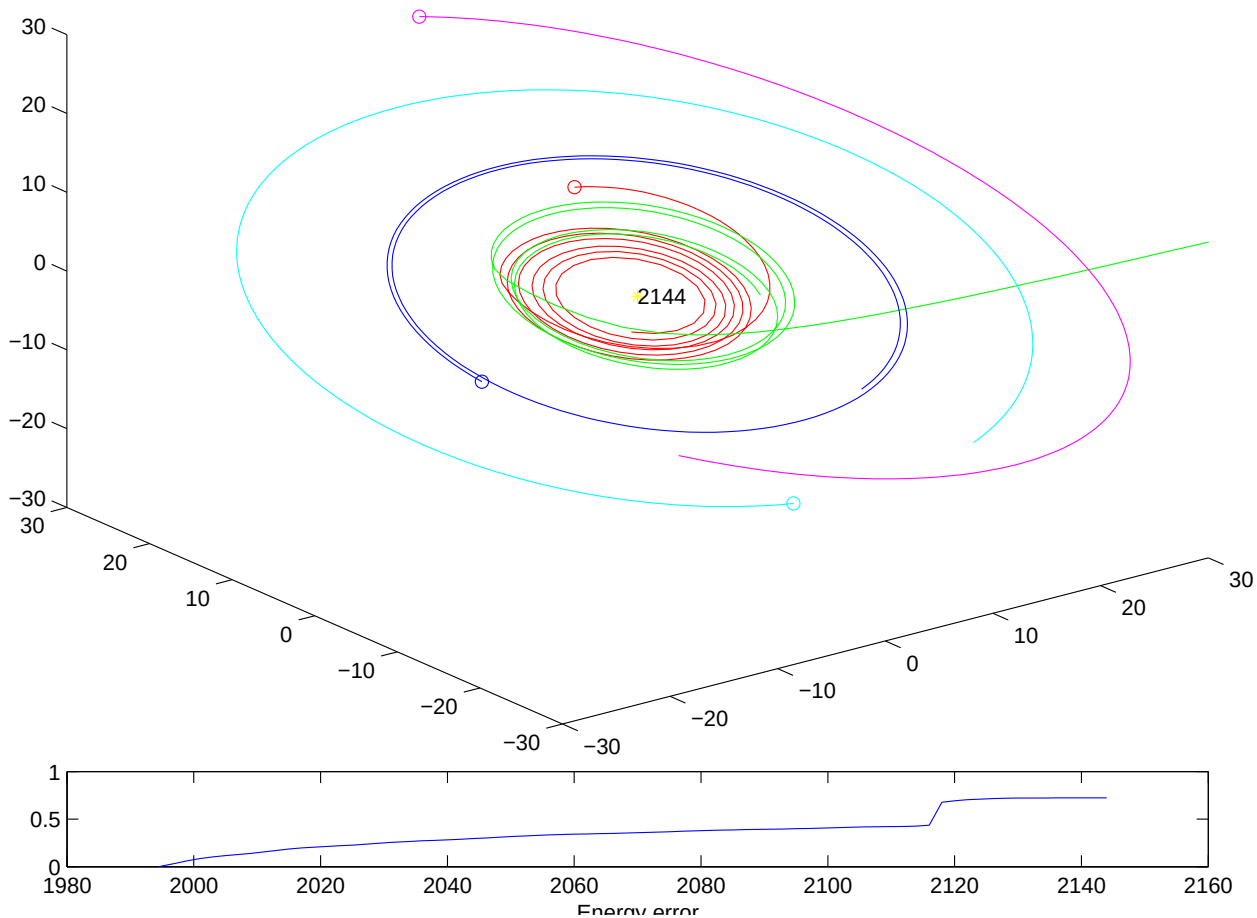
$$\mathbf{q}_{k+1} = \mathbf{q}_k + h\dot{\mathbf{q}}(\mathbf{q}_{k+1}, \mathbf{p}_{k+1}),$$
$$\mathbf{p}_{k+1} = \mathbf{p}_k + h\dot{\mathbf{p}}(\mathbf{q}_{k+1}, \mathbf{p}_{k+1}).$$

- Symplectic Euler

$$\mathbf{q}_{k+1} = \mathbf{q}_k + h\dot{\mathbf{q}}(\mathbf{q}_k, \mathbf{p}_{k+1}),$$
$$\mathbf{p}_{k+1} = \mathbf{p}_k + h\dot{\mathbf{p}}(\mathbf{q}_k, \mathbf{p}_{k+1}).$$

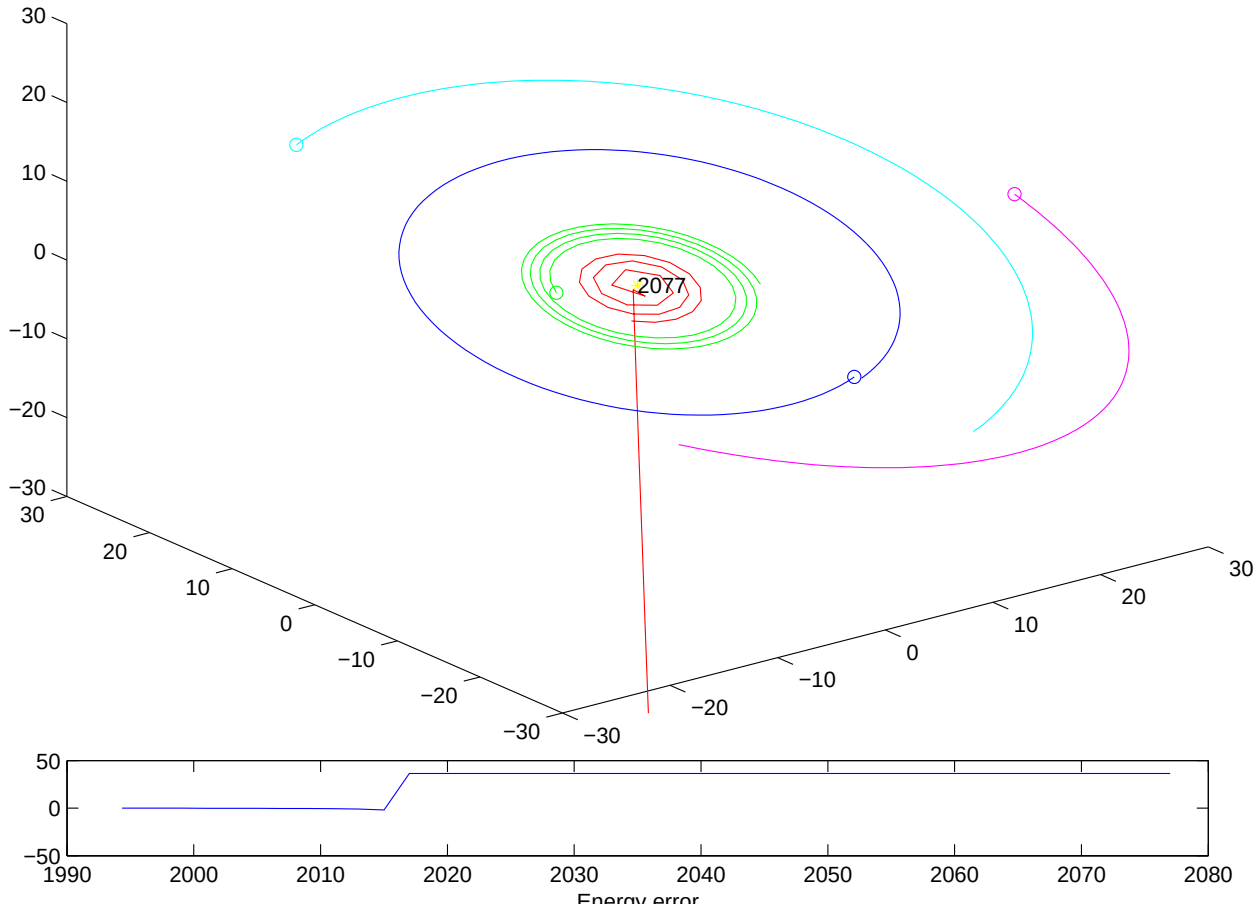
Geometric Integration: Energy Stability

Forward Euler



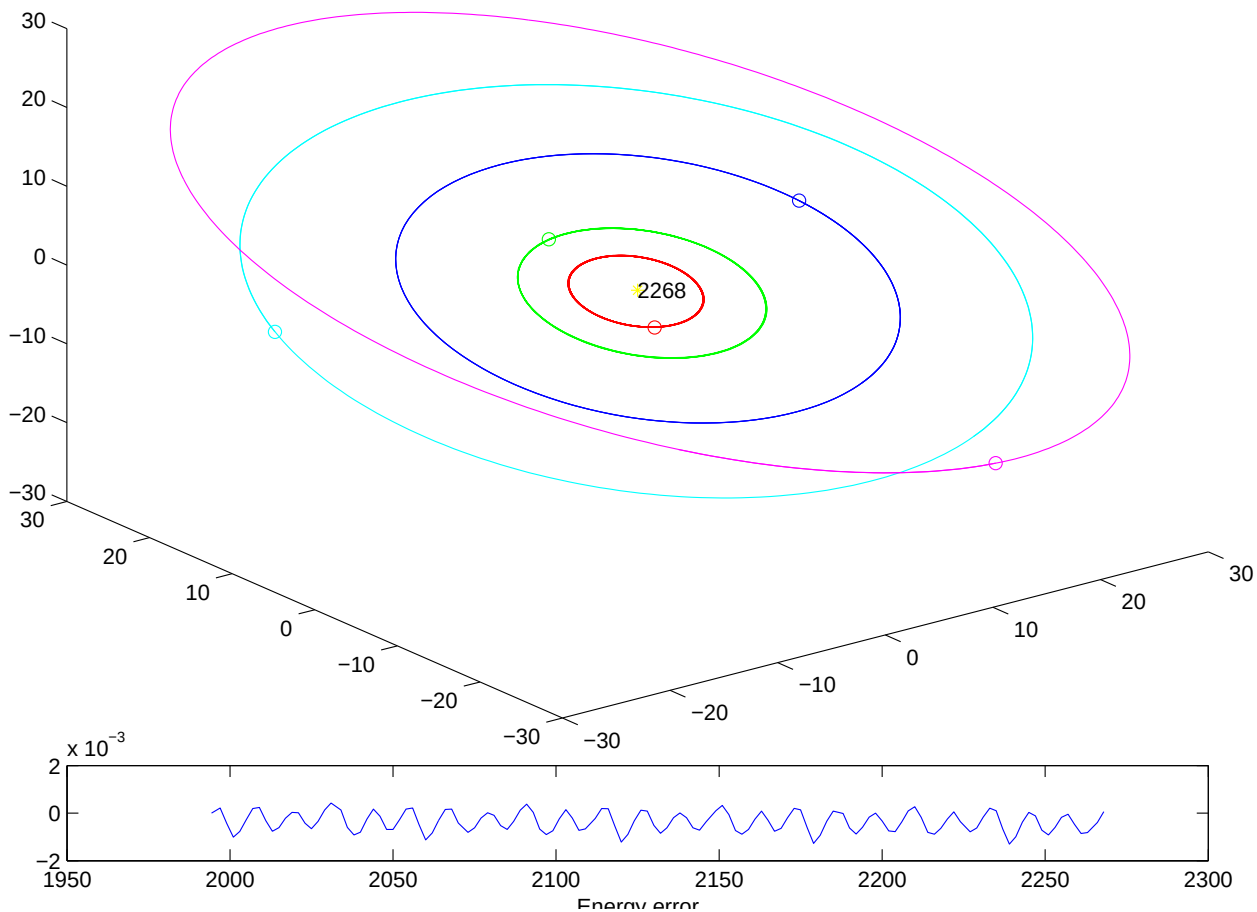
Geometric Integration: Energy Stability

Inverse Euler



Geometric Integration: Energy Stability

Symplectic Euler



Introduction to Computational Geometric Mechanics

Geometric Mechanics

- Differential geometric and symmetry techniques applied to the study of Lagrangian and Hamiltonian mechanics.

Computational Geometric Mechanics

- Constructing computational algorithms using ideas from geometric mechanics.
- Variational integrators based on discretizing Hamilton's principle, automatically symplectic and momentum preserving.

Introduction to Computational Geometric Mechanics

Why adopt this approach?

- Provides a systematic framework to construct structure-preserving numerical schemes that are consistent with the underlying geometry of the problem.
- Structure-preservation can be important from the point of view of stability, accuracy, and efficiency.
- Provides insight into the discrete analogues of differential geometric structures that are preserved by numerical schemes.

Discrete Mechanics

Traditional Approach

- Discretization is performed at the level of the equation, for example, finite-differences and finite-elements applied to the differential equations of motion.

Alternative Approach

- Discretize underlying variational principles.

Continuous Mechanics

Lagrangian Formulation of Mechanics

- Given a Lagrangian $L : TQ \to \mathbb{R}$, the solution curve satisfies **Hamilton's variational principle**,

$$\delta \int_{t_0}^{t_1} L\left(q\left(t\right), \dot{q}\left(t\right)\right) dt = 0.$$

- This is equivalent to the **Euler-Lagrange equation**,

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0.$$

- When the Lagrangian has the form $L = \frac{1}{2}\dot{q}^T M \dot{q} - V\left(q\right)$, this reduces to Newton's Second Law,

$$\frac{d}{dt}\left(M\dot{q}\right) = -\frac{\partial V}{\partial q}.$$

Discrete Mechanics

Discretization of Mechanics

- Approximate TQ by $Q \times Q$. Diagonal group action of G on $Q \times Q$
- The **discrete Lagrangian** $L_d : Q \times Q \to \mathbb{R}$ is a generating function of the discrete flow. A particularly simple choice of discrete Lagrangian is given by,

$$L_d\left(q_k, q_{k+1}\right) = h \cdot L\left(\frac{q_{k+1} + q_k}{2}, \frac{q_{k+1} - q_k}{h}\right)$$

- Consider the **discrete action sum** $\mathbb{S} : Q^{N+1} \to \mathbb{R}$ defined by

$$\mathbb{S} = \sum_{k=0}^{N-1} L_d\left(q_k, q_{k+1}\right).$$

which is a discrete analogue of the action integral.

Discrete Mechanics

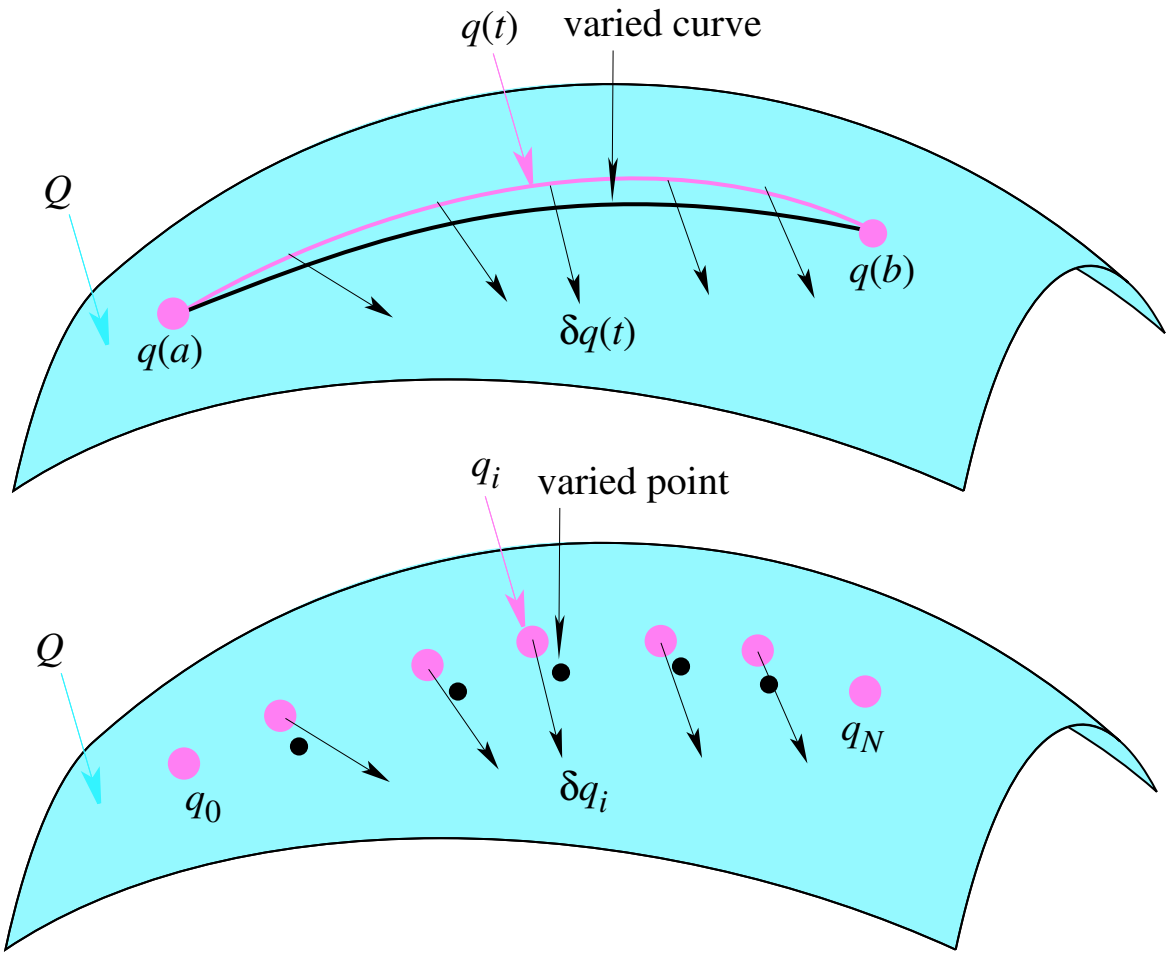
Discrete Variational Principle

- Hamilton's variational principle states that the solution curve has an action integral that is stationary.
- Analogously, the **discrete variational principle** states that,

$$\delta \sum_{k=0}^{N-1} L_d\left(q_k, q_{k+1}\right) = 0.$$

Discrete Mechanics

Discrete Variational Principle



Discrete Mechanics

Discrete Euler-Lagrange equation

- To extremize $\mathbb{S}$ over $q_0, \cdots, q_N$, we set

$$\frac{\partial \mathbb{S}}{\partial q_k} = 0, \quad k = 0, \ldots, N.$$

This implies,

$$D_1 L_d\left(q_k, q_{k+1}\right) \delta q_k + D_2 L_d\left(q_{k-1}, q_k\right) \delta q_k = 0, \quad k = 1, \ldots, N-1.$$

Since $\delta q_0 = \delta q_N = 0$ and the rest of the variations are arbitrary, we obtain the **discrete Euler-Lagrange** equation,

$$D_1 L_d \circ \Phi + D_2 L_d = 0.$$

Correspondance between discrete and continuous mechanics

- Consider the **exact discrete Lagrangian** given by,

$$L_d\left(q_k, q_{k+1}\right) = \int_{t_k}^{t_{k+1}} L\left(q\left(t\right), \dot{q}\left(t\right)\right) dt$$

  where $q : [t_k, t_{k+1}] \to Q$ is a solution of the Euler-Lagrange equations for L which satisfies the boundary conditions $q\left(t_k\right) = q_k$ and $q\left(t_{k+1}\right) = q_{k+1}$.

- This choice is motived by the **Jacobi solution** of Hamilton-Jacobi Theory, where the action integral is a generating function of the Hamiltonian flow.

Correspondance between discrete and continuous mechanics.

- Can show that with the exact discrete Lagrangian, the discrete curve $\{q_k\}_{k=0}^{n}$ satisfying the Discrete Euler-Lagange equations discretely sample the continuous solution curve $q(t)$ of the Euler-Lagrange equations for the corresponding Lagrangian.

$$q_k = q\left(t_k\right)$$

- In practice, the exact discrete Lagrangian, like Jacobi's solution, cannot be computed exactly. As such, numerical quadrature methods are used to approximate the exact discrete Lagrangian.
- Can be shown that a discrete Lagrangian given by an n-th order accurate quadrature method yields an n-th order accurate symplectic integrator. This recovers a class of previously discovered Symplectic Partitioned Runger-Kutta methods.

Canonical Symplectic Structure

Hamilton's Canonical Equations

$$\dot{q}^i = \frac{\partial H}{\partial p_i}$$
$$\dot{p}_i = -\frac{\partial H}{\partial q^i}$$

- If we adopt the coordinate system, $z = (q, p)$, the **Canonical Symplectic Form**, $\Omega = dp_i \wedge dq^i$ has the matrix representation given by:

$$\mathbb{J} = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix}$$

- Hamilton's equations, $\dot{z} = X_H = \mathbb{J}\nabla H$ can be written as:

$$\Omega\left(X_H(z), v\right) = dH.z$$

Discrete Symplectic Structure

Fiber Derivative

$$\mathbb{F}L_d : Q \times Q \to T^*Q$$

$$(q_0, q_1) \mapsto (q_0, D_1 L_d (q_0, q_1))$$

Discrete Symplectic Form

$$\begin{aligned}
\omega_L &= (\mathbb{F}L_d)^* (\Omega_L) \\
&= d\left((\mathbb{F}L_d)^* \left(-p_i dq^i\right)\right) \\
&= d\left(-\frac{\partial L_d}{\partial q_k^i}(q_k, q_{k+1})\right) dq_k^i \\
&= \frac{\partial^2 L_d}{\partial q_k^i \partial q_{k+1}^j}(q_k, q_{k+1})\, dq_k^i \wedge dq_{k+1}^j
\end{aligned}$$

Momentum Maps

Continuous Momentum Map

- A momentum map $J : T^*Q \to \mathfrak{g}^*$ is a generalization of the familar conjugate momentum in Hamiltonian mechanics.
- Given a mechanical system that is invariant under the action of the Lie group G on the configuration manifold Q, we define a momentum map by,

$$\left\langle J\left(\alpha_q\right), \xi\right\rangle \equiv \left\langle \alpha_q, \xi_Q(q)\right\rangle$$

Discrete Momentum Map

- **Discrete Momentum Map** $J_d : Q \times Q \to \mathfrak{g}^*$,

$$\left\langle J_d\left(q_k, q_{k+1}\right), \xi\right\rangle \equiv \left\langle D_1 L_d\left(q_k, q_{k+1}\right), \xi_Q\left(q_k\right)\right\rangle$$

Momentum Maps

Example: Angular Momentum

Let $SO(3)$ act on $\mathbb{R}^3$ by matrix multiplication.

$$\mathbf{A} \cdot \mathbf{q} = \mathbf{A}\mathbf{q}$$

The infinitesimal generator is given by $\hat{\omega}_{\mathbb{R}^3}(\mathbf{q}) = \hat{\omega}\mathbf{q} = \omega \times \mathbf{q}$, where $\omega \in \mathbb{R}^3$. The momentum map $J : T^*\mathbb{R}^3 \to \mathfrak{so}(3)^* \cong \mathbb{R}^3$ is given by,

$$\langle J(\mathbf{q}, \mathbf{p}), \omega \rangle = \mathbf{p} \cdot \hat{\omega}\mathbf{q} = \omega \cdot (\mathbf{q} \times \mathbf{p}),$$

that is,

$$J(\mathbf{q}, \mathbf{p}) = \mathbf{q} \times \mathbf{p},$$

which is the familiar expression for angular momentum.

Discrete Mechanics

What does this way of thinking buy you?

- Systematic method of constructing symplectic-momentum integrators of arbitrarily high-order.
- In contrast to non-constructive condition on the coefficients of the partitioned Runge–Kutta scheme:

$$\begin{aligned} b_i \tilde{a}_{ij} + \tilde{b}_j a_{ji} &= b_i \tilde{b}_j, & i, j &= 1, \ldots, s, \\ b_i &= \tilde{b}_i, & i &= 1, \ldots s. \end{aligned}$$

- Naturally leads to generalized schemes such as Lie group, multi-scale, and pseudospectral variational integrators.

Comparing representations of the rotation group

Euler Angles

- Local coordinate chart, exhibits singularities.
- Requires change of charts to simulate large attitude maneuvers.

Unit Quaternions

- Reprojection used to stay on unit 3-sphere.
- The 3-sphere is a double-cover of $SO(3)$ which causes topological problems for optimization.

Rotation Matrices

- 9 dimensional space (3×3 matrices) with a 6 dimensional constraint (orthogonality), but the exponential map saves the day.

Variational Lie Group Techniques

Basic Idea

- To stay on the Lie group, we parametrize the curve by the initial point g_0, and elements of the Lie algebra ξ_i, such that,

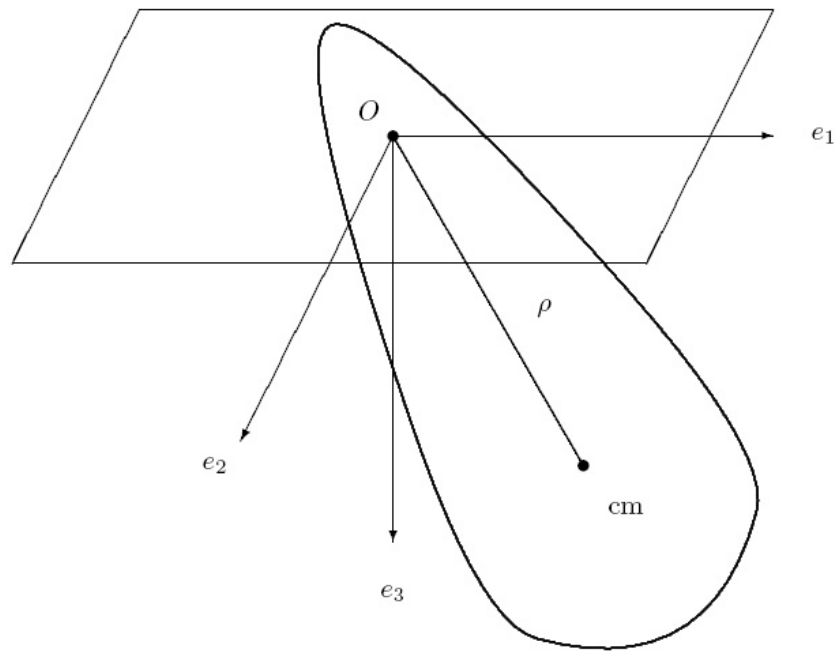
$$g_d(t) = \exp\left(\sum \xi^s \tilde{l}_{\kappa,s}(t)\right) g_0$$

- This involves standard interpolatory methods on the Lie algebra that are lifted to the group using the exponential map.
- Automatically stays on $SO(n)$ without the need for reprojection, constraints, or local coordinates.
- Order of accuracy of method is independent of the retraction, as the variational principle is at the level of the Lie group, and the retraction is simply used to locally parametrize the group.

Model Problem

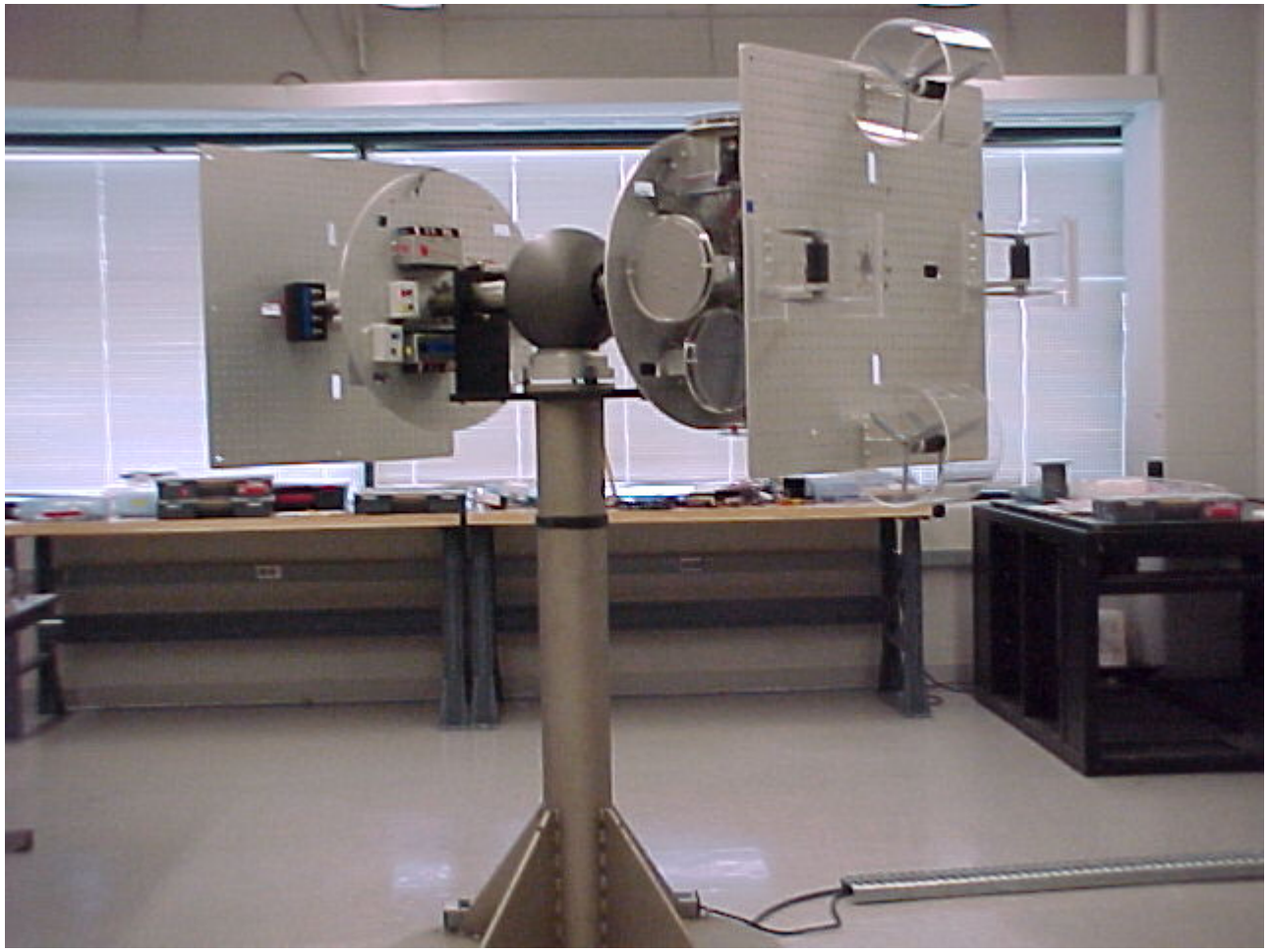
3D Pendulum

- A rigid body, with a pivot point and a center of mass that are not collocated, under gravitational forces.
- Three degrees of freedom.
- Exhibits surprisingly rich and complex dynamics.



Physical Realization of a 3D Pendulum

Triaxial Attitude Control Testbed



Attitude Dynamics and Control Laboratory, University of Michigan, Ann Arbor.

Example of a Lie Group Variational Integrator

3D Pendulum

- **Lagrangian**

$$L(R,\omega) = \frac{1}{2}\int_{Body} \|\widehat{(\tilde{\rho})}\omega\|^2 dm - V(R),$$

where $\widehat{\cdot} : \mathbb{R}^3 \rightarrow \mathbb{R}^{3\times 3}$ is a skew mapping such that $\widehat{x}y = x \times y$.

- **Equations of motion**

$$J\dot{\omega} + \omega \times J\omega = M,$$

where $\widehat{M} = \frac{\partial V}{\partial R}^T R - R^T \frac{\partial V}{\partial R}$.

$$\dot{R} = R\widehat{\omega}.$$

Example of a Lie Group Variational Integrator

3D Pendulum

- **Discrete Lagrangian**

$$L_d(R_k, F_k) = \frac{1}{h}\,\mathrm{tr}\left[(I_{3\times 3} - F_k)J_d\right] - \frac{h}{2}V(R_k) - \frac{h}{2}V(R_{k+1}).$$

- **Discrete Equations of Motion**

$$\begin{aligned} J\omega_{k+1} &= F_k^T J\omega_k + hM_{k+1}, \\ S(J\omega_k) &= \frac{1}{h}\left(F_k J_d - J_d F_k^T\right), \\ R_{k+1} &= R_k F_k. \end{aligned}$$

Example of a Lie Group Variational Integrator

Automatically staying on the rotation group

- The magic begins with the ansatz,

$$F_k = \exp(\widehat{f_k}),$$

and the Rodrigues' formula, which converts the equation,

$$\widehat{J\omega_k} = \frac{1}{h}\left(F_k J_d - J_d F_k^T\right),$$

into

$$hJ\omega_k = \frac{\sin\|f_k\|}{\|f_k\|}\, Jf_k + \frac{1-\cos\|f_k\|}{\|f_k\|^2}\, f_k \times Jf_k.$$

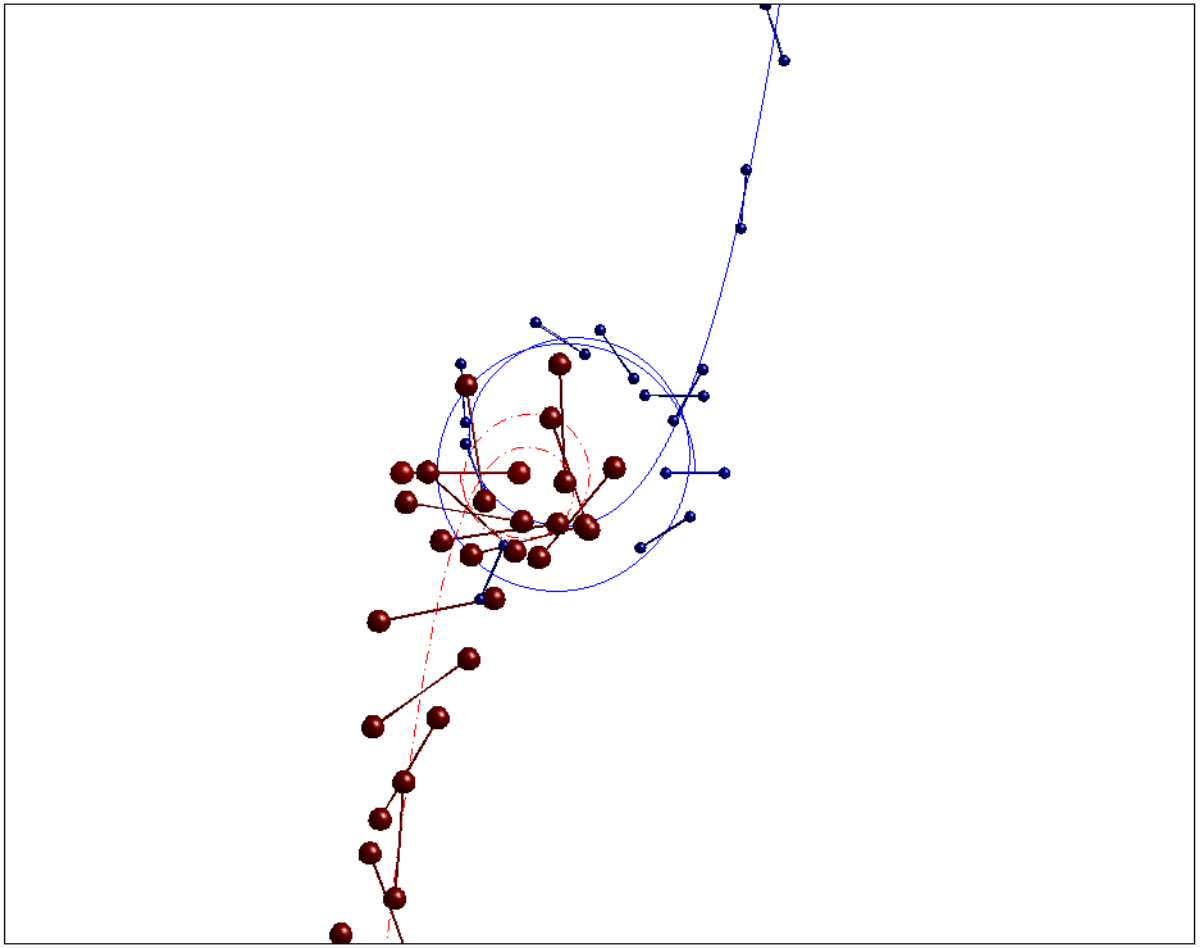
- Since F_k is the exponential of a skew matrix, it is a rotation matrix, and by matrix multiplication $R_{k+1} = R_k F_k$ is a rotation matrix.

Numerical Simulation

- **Chaotic Motion of a 3D Pendulum**

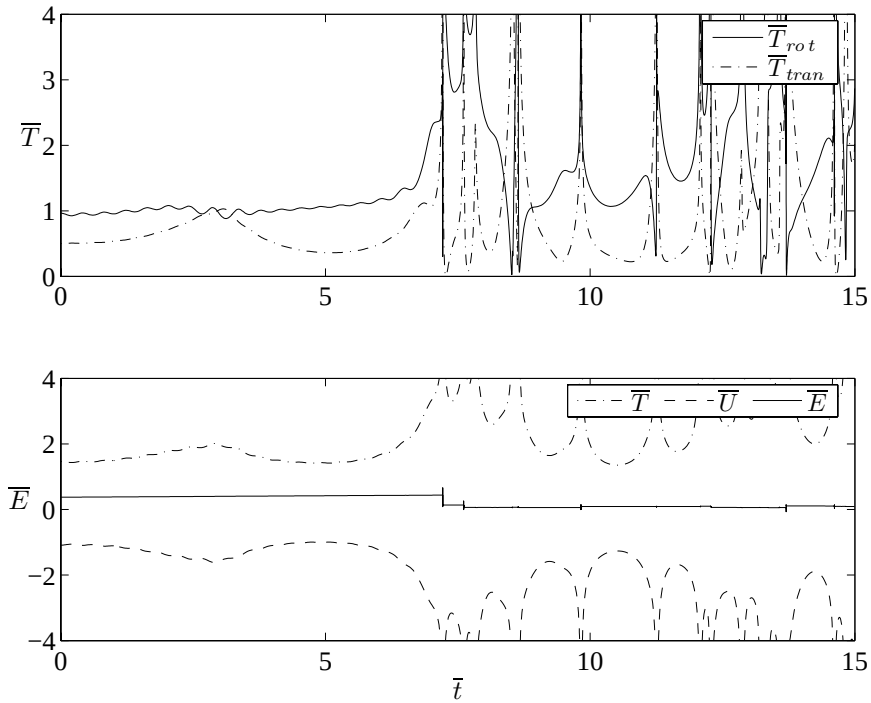
Numerical Simulations

- **Flyby of two dumbbells**

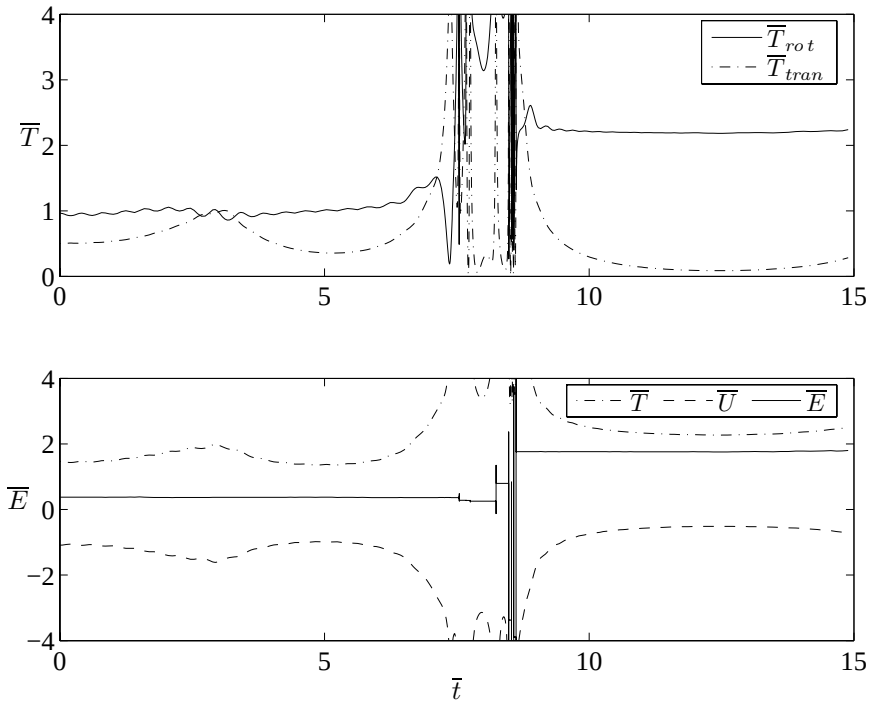


Numerical Simulations

Effect of representations (Runge-Kutta)



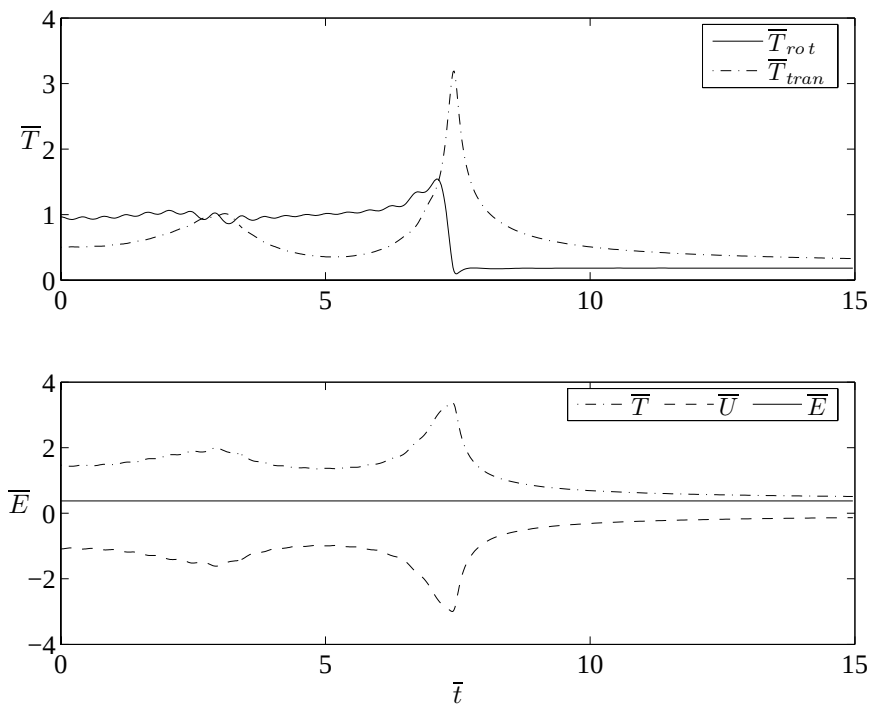
Runge-Kutta with quaternions



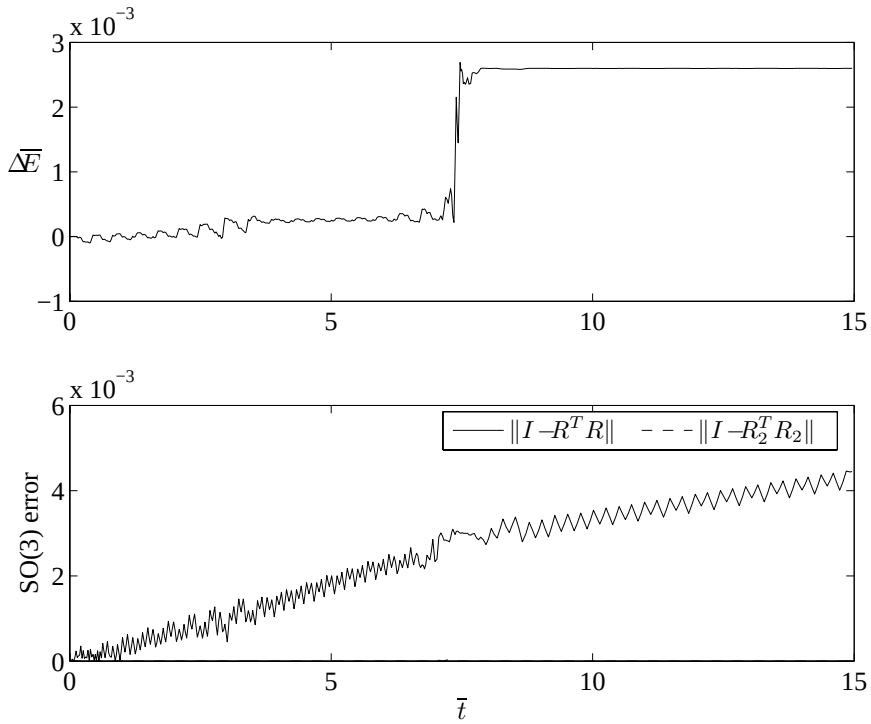
Runge-Kutta with Euler angles

Numerical Simulations

Effect of representations (Runge-Kutta)



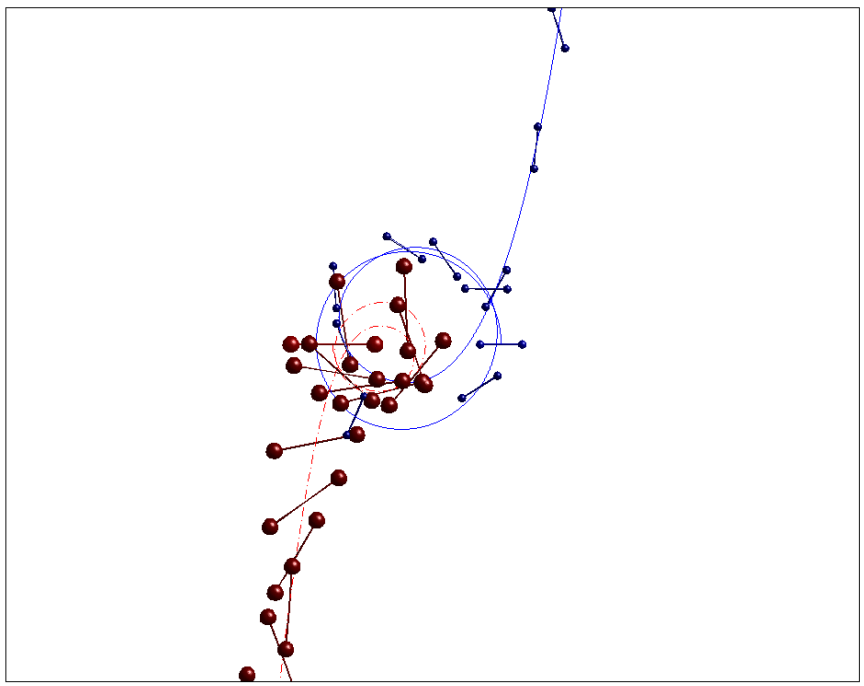
Runge-Kutta with SO(3)



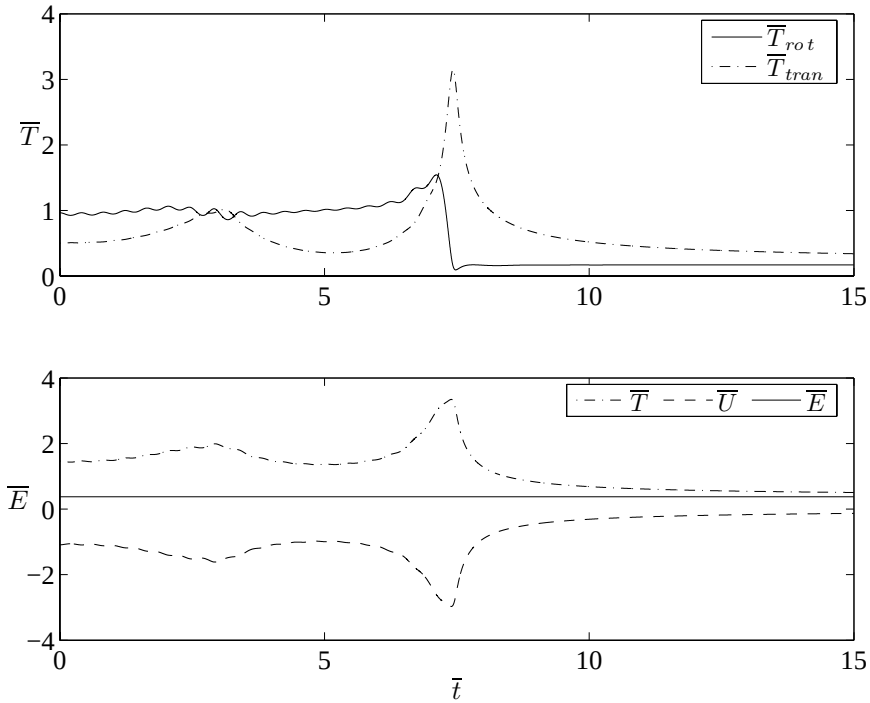
Runge-Kutta with SO(3) (Integration error)

Numerical Simulations

Lie group variational integrator on $\mathrm{SO}(3)$



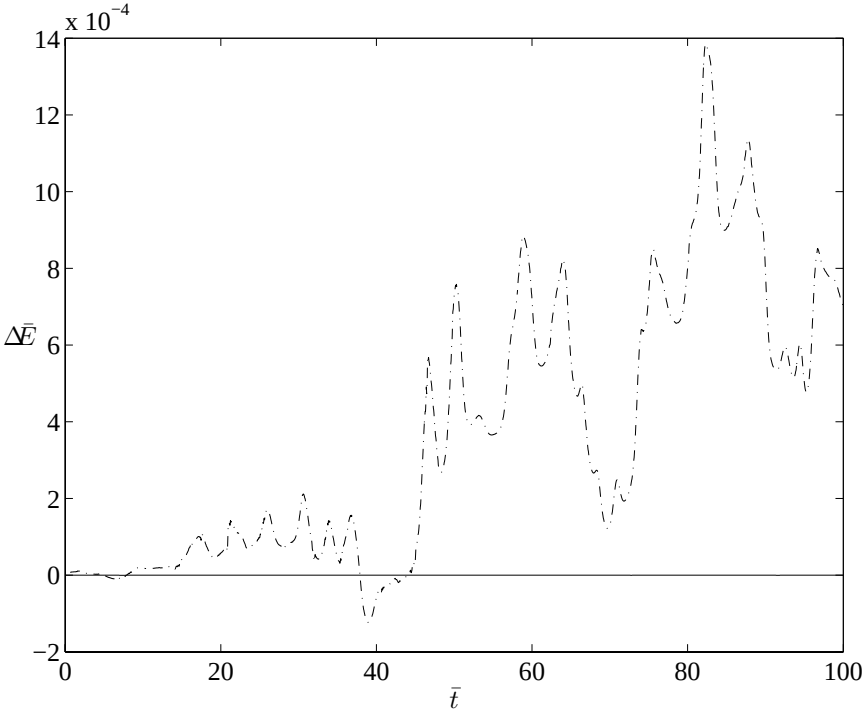
Trajectory in inertial frame



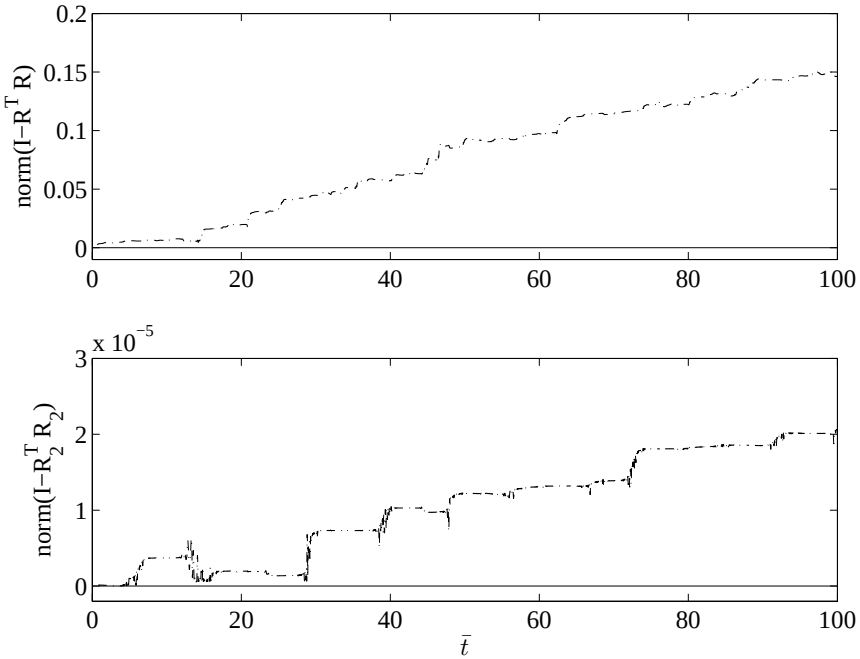
Transfer of energy

Numerical Simulations

Conservation Properties: Lie Group Integrator



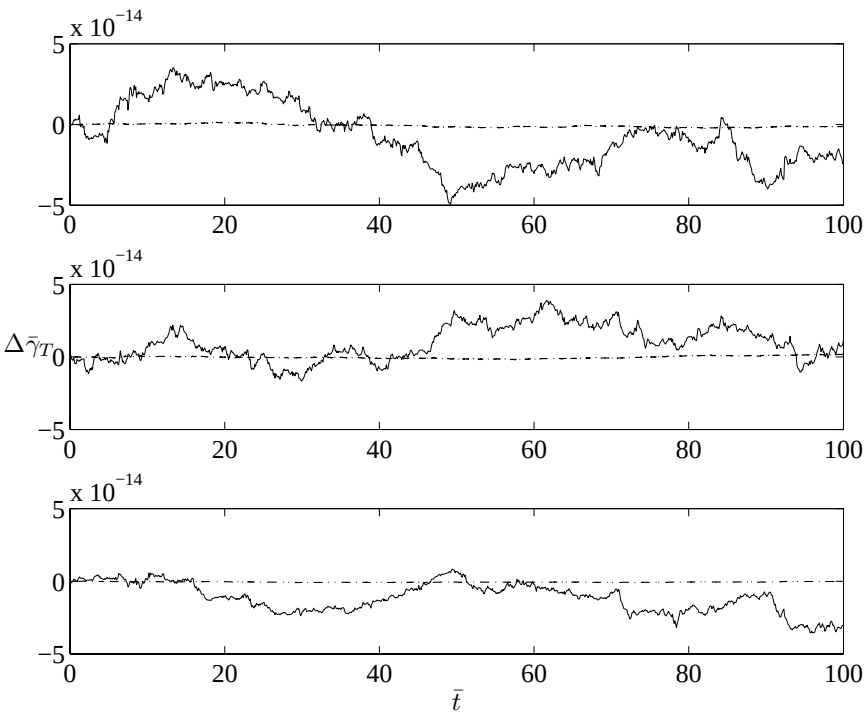
deviation in total energy



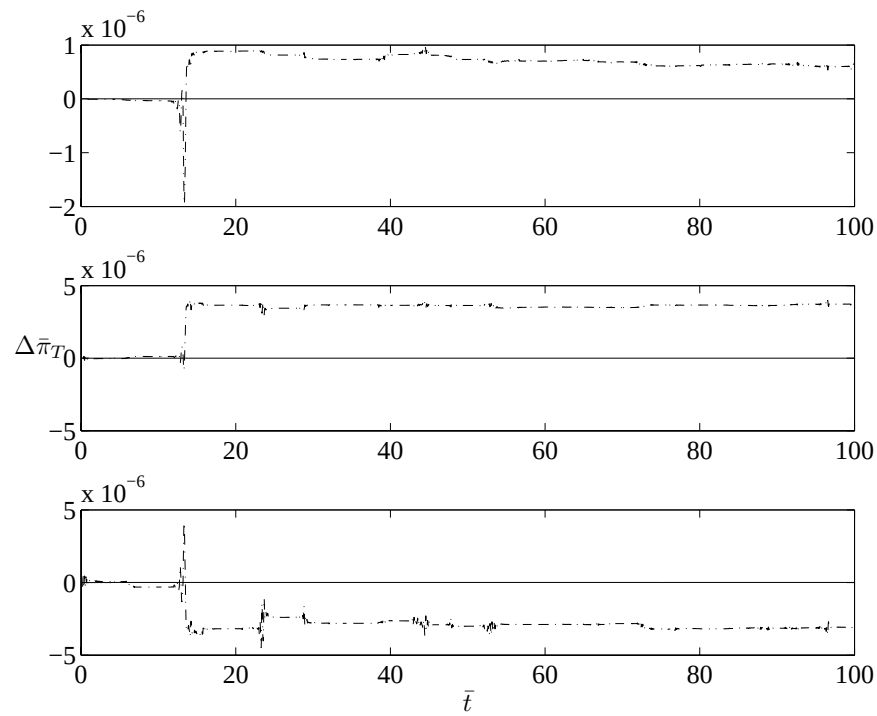
error in the rotation matrix

Numerical Simulations

Conservation Properties: Lie Group Integrator



deviation in total linear momentum



deviation in total angular momentum

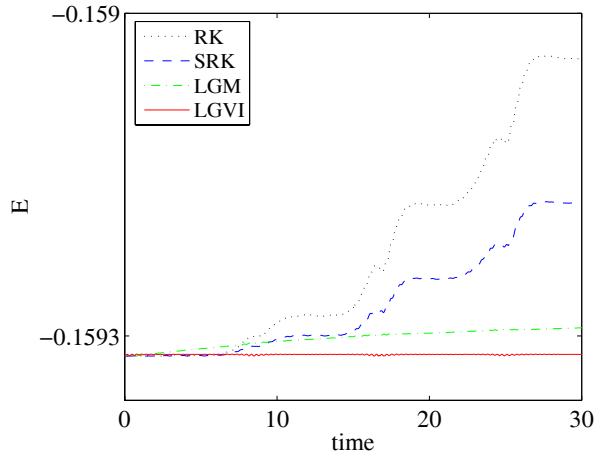
Numerical Simulations

Comparison with other methods

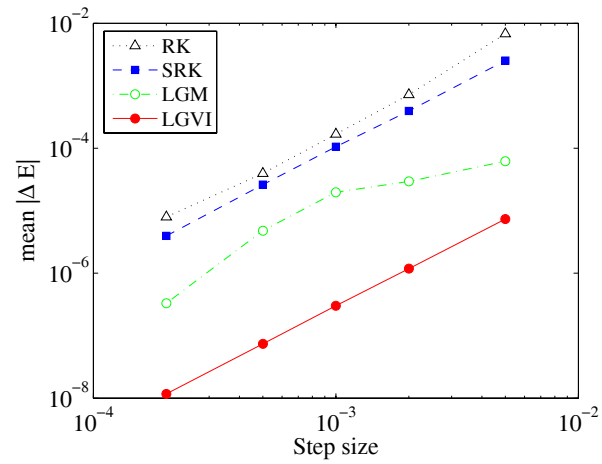
- Our Lie group variational integrator (LGVI) is a **Lie Störmer–Verlet** method, so it is a second-order symplectic Lie group method.
- We compare it to other second-order accurate methods:
  - **Explicit Midpoint Rule (RK):**
    Preserves neither symplectic nor Lie group properties.
  - **Implicit Midpoint Rule (SRK):**
    Symplectic but does not preserve Lie group properties.
  - **Crouch-Grossman (LGM):**
    Lie group method but not symplectic.

Numerical Simulations

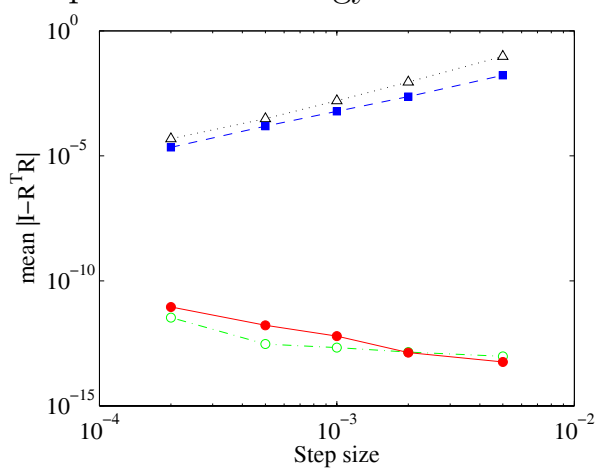
Comparison with other methods



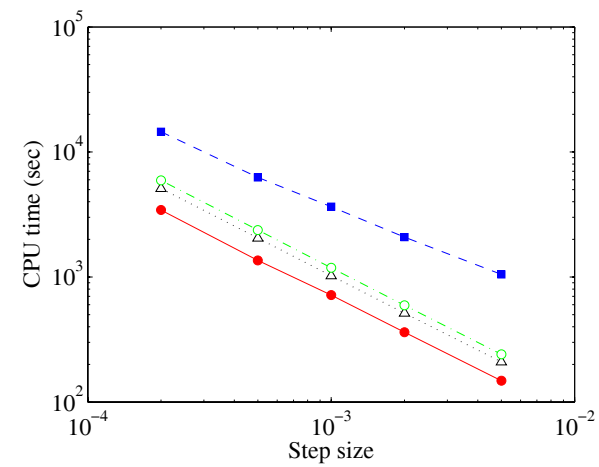
Computed total energy for 30 seconds



Mean total energy error $|E - E_0|$ vs. step size



Mean orthogonality error $\|I - R^T R\|$ vs. step size



CPU time vs. step size

Applications to Asteroid Simulations

Computational Considerations

- Asteroids are approximated by rubble piles (hard sphere models) or simplicial complexes.
- Force evaluations using fast multipole methods or polyhedral potential techniques.
- Computational cost is dominated by cost of force evaluation.
- Lie Störmer–Verlet variational integrators use only one force evaluation per timestep, and are only implicit in the attitude, and converge in 2-3 Newton steps.
- Used by Scheeres, et al. to accurately simulate binary near-Earth Asteroid 66391 (1999 KW4).

Applications to Asteroid Simulations

Numerically implementing geometric control algorithms

Traditional approach

- Local analysis of the connection near the desired shape position.
- Gives a closed form expression for the geometric phase associated with infinitesimally small loops in shape space.
- Resulting shape trajectories are often suboptimal and slow.

Alternative approach

- Homotopy-based optimal control algorithm using geometrically exact numerical schemes.
- Allows for large-amplitude trajectories that are global in nature, and more efficient than infinitesimal loops.

Discrete Optimal Control

Essential Ideas

- Use the **discrete Lagrange–d'Alembert** principle,

$$\delta \sum L_d\left(q_k, q_{k+1}\right) + \sum F_d\left(q_k, q_{k+1}\right) \cdot \left(\delta q_k, \delta q_{k+1}\right) = 0,$$

  to derive the **discrete forced Euler–Lagrange** equations, and impose these as **constraints at every time-step**.

- This yields **greater fidelity** to the equations of motion that imposing the dynamical constraints using the method of collocation.

- The resulting numerical solutions are **group equivariant**, which implies that the numerical solutions are independent of the choice of coordinate frame.

Shooting based optimization using variational integrators

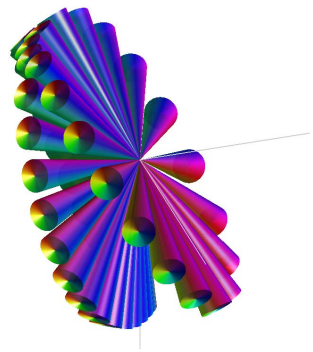
General approach

- Relax terminal boundary conditions, and guess initial control torque.
- Evolve attitude and control torques using equations of motion and optimality conditions.
- Compute sensitivity of terminal boundary conditions on initial control torques, and iterate to convergence.

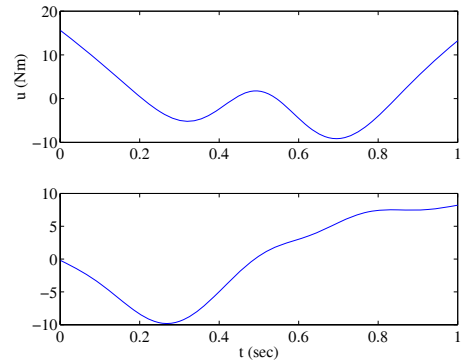
Robust computation of sensitivities

- Structure preserving properties of the variational integrator allow the robust computation of sensitivities.
- Problems considered do not appear to require multiple shooting to achieve convergence.

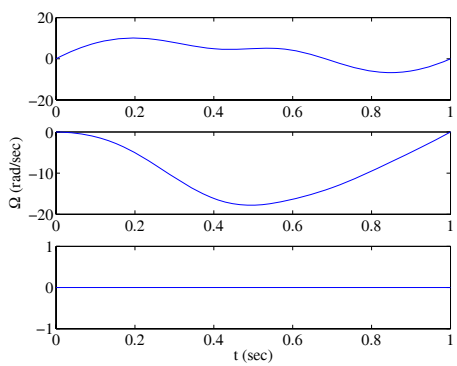
Under-actuated control of a 3D pendulum



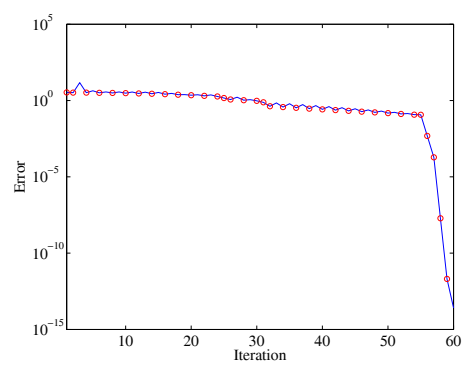
Attitude Maneuver



Control input u

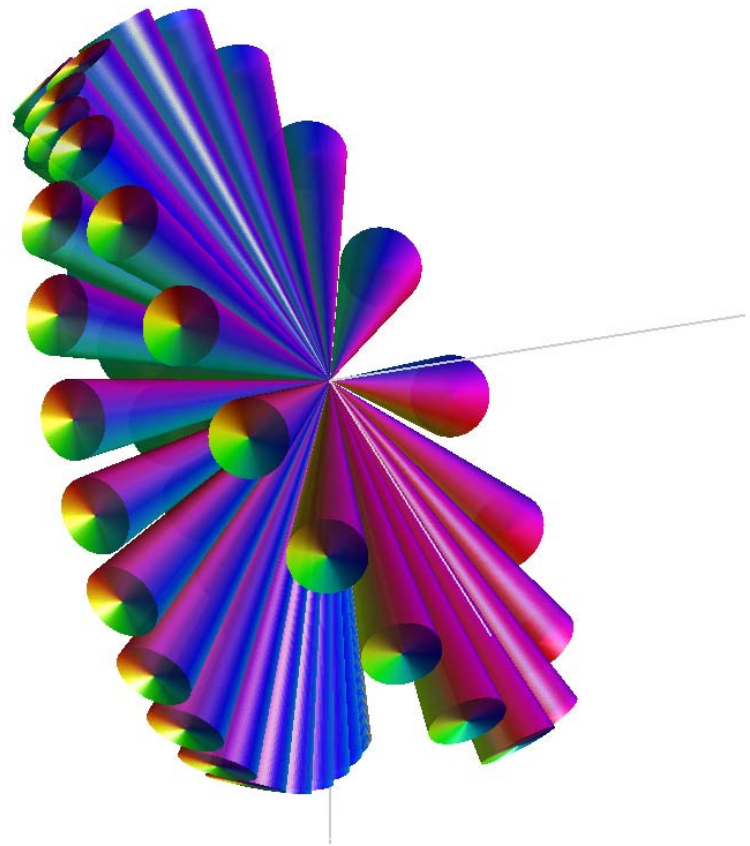


Angular velocity Ω

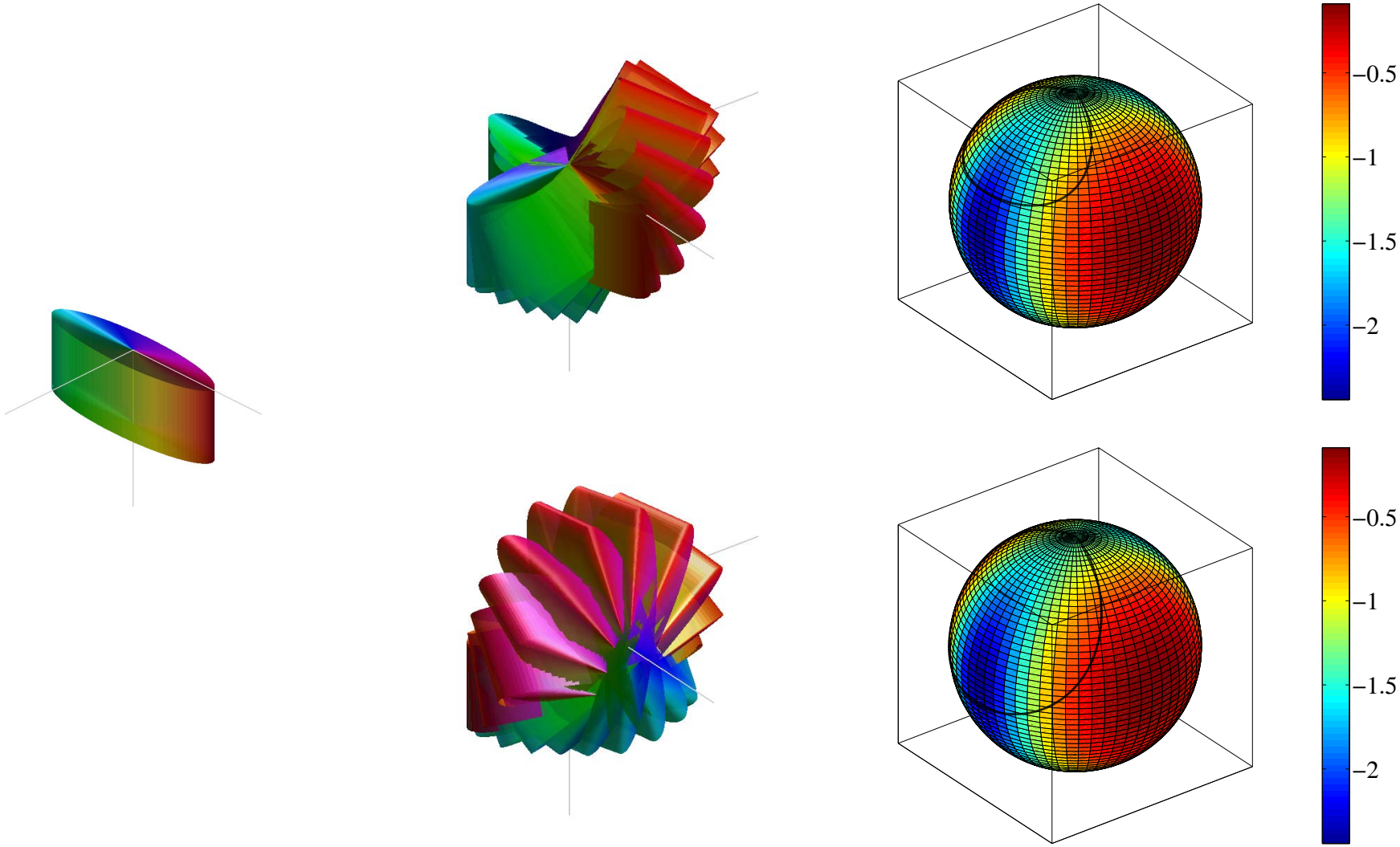


Convergence rate

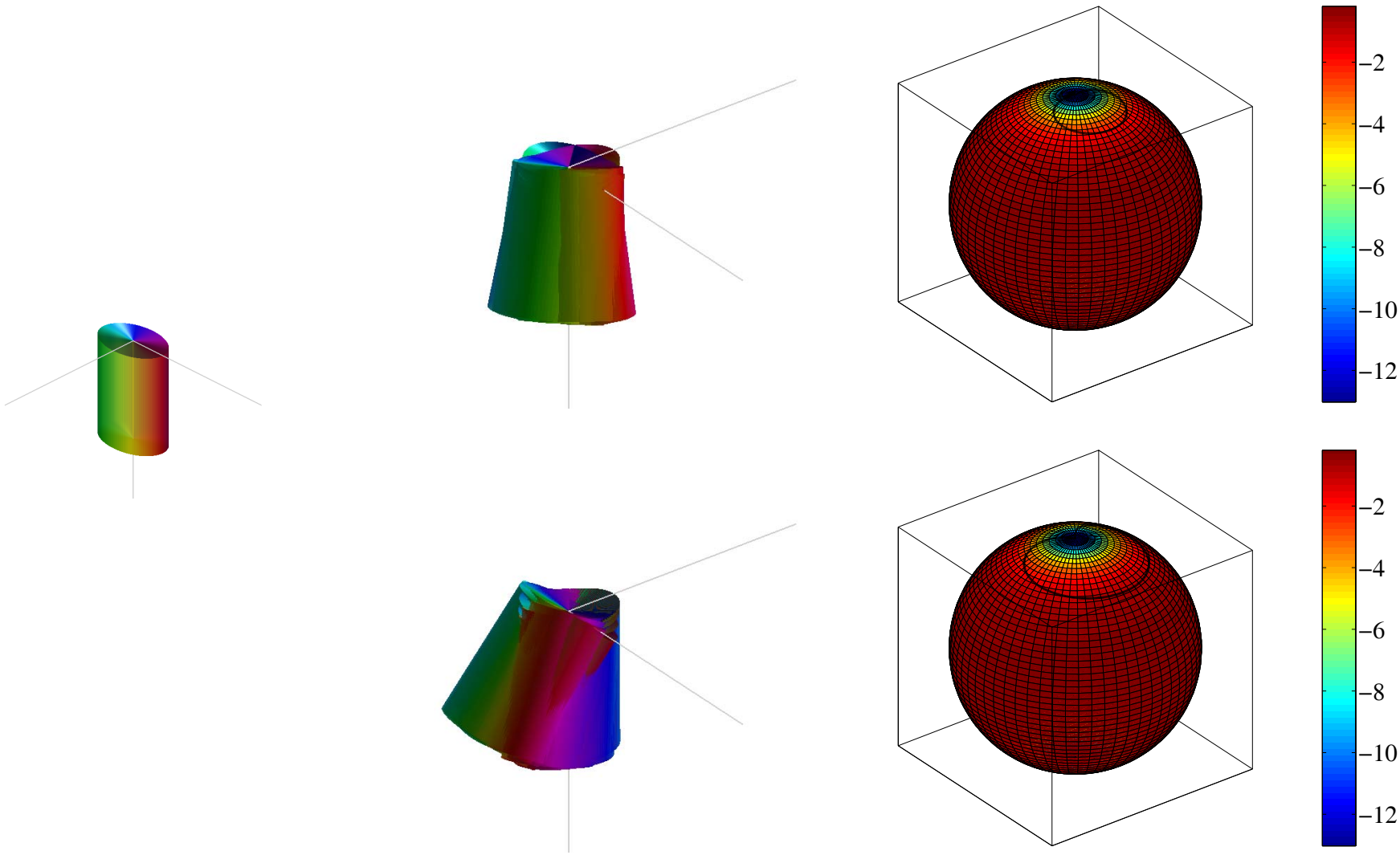
Under-actuated control of a 3D pendulum



Under-actuated control with symmetry of a 3D pendulum



Under-actuated control with symmetry of a 3D pendulum



Variational Integrators on S^2

Constrained variations

- The condition that $q \in S^2 = \{q \in \mathbb{R}^3 | q \cdot q = 1\}$ yields a **constrained variation** of q in the variational principle.

$$\delta q = \xi \times q,$$

where $\xi \in \mathbb{R}^3$ is constrained to be orthogonal to q, i.e., $\xi \cdot q = 0$.

Lagrangian

- The configuration space is a cartesian product of two-spheres, $Q = (S^2)^n$, and the Lagrangian has the form,

$$L(q_1, \ldots, q_n, \dot{q}_1, \ldots, \dot{q}_n) = \frac{1}{2} \sum_{i,j=1}^{n} \dot{q}_j^T M_{ij} \dot{q}_i - V(q_1, \ldots, q_n),$$

Variational Integrators on S^2

Spherical Pendulum

$$
\begin{aligned}
r_{k+1} =& \left(h\omega_k + \frac{h^2 g}{2l} r_k \times e_3\right) \times r_k + r_k \sqrt{1 - \left\| h\omega_k + \frac{h^2 g}{2l} r_k \times r_3 \right\|^2} \\
\omega_{k+1} =& \omega_k + \frac{hg}{2l} r_k \times e_3 + \frac{hg}{2l} r_{k+1} \times e_3
\end{aligned}
$$

Double Spherical Pendulum

$$
\begin{bmatrix} \frac{2}{1+f_1\cdot f_1} I_{3\times 3} & -\frac{2\alpha}{1+f_2\cdot f_2}\hat{r}_1\hat{r}_2 \\ -\frac{2\beta}{1+f_1\cdot f_1}\hat{r}_2\hat{r}_1 & \frac{2}{1+f_2\cdot f_2} I_{3\times 3} \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \begin{bmatrix} h\omega_{1_k} - h\alpha(r_{1_k} \times (r_{2_k} \times \omega_{2_k})) + \frac{h^2 g}{2l_1}(r_{1_k} \times e_3) + \frac{2\alpha f_2\cdot f_2}{1+f_2\cdot f_2}\hat{r}_1 r_2 \\ h\omega_{2_k} - h\beta(r_{2_k} \times (r_{1_k} \times \omega_{1_k})) + \frac{h^2 g}{2l_2}(r_{2_k} \times e_3) + \frac{2\beta f_1\cdot f_1}{1+f_1\cdot f_1}\hat{r}_2 r_1 \end{bmatrix}
$$

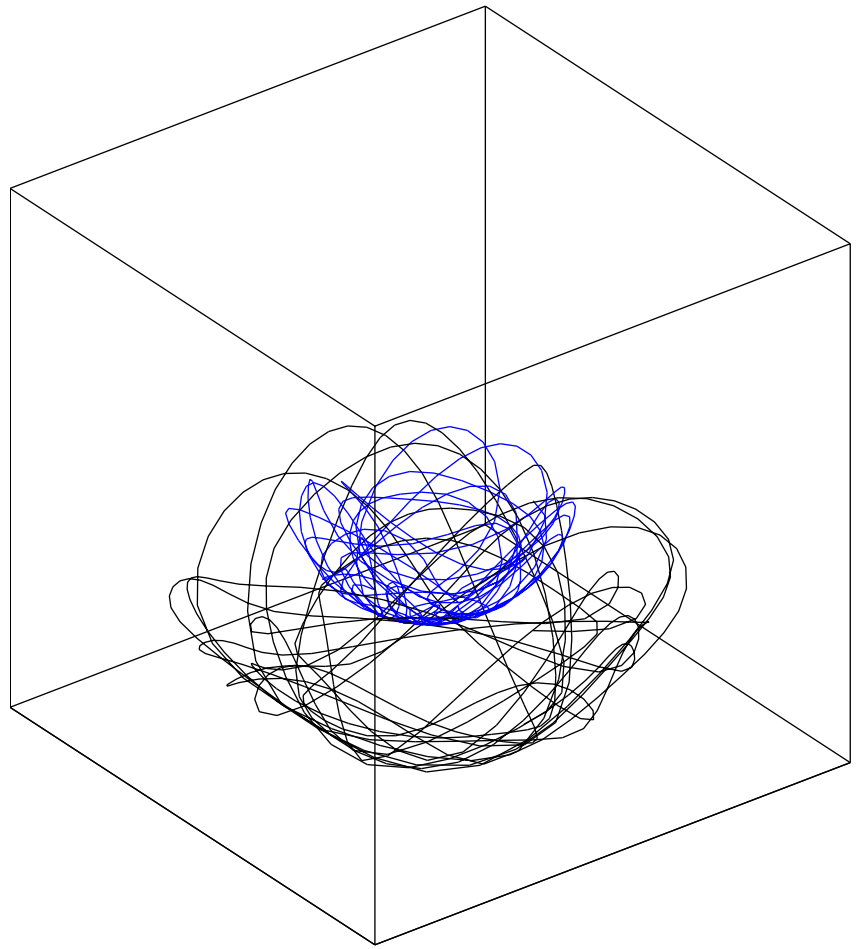
$$
\begin{aligned}
r_{1_{k+1}} &= (I_{3\times 3} + \hat{f}_1)(I_{3\times 3} - \hat{f}_1)^{-1} r_{1_k} \\
r_{2_{k+1}} &= (I_{3\times 3} + \hat{f}_2)(I_{3\times 3} - \hat{f}_2)^{-1} r_{2_k}
\end{aligned}
$$

where $\alpha = \frac{m_2}{m_1+m_2}\frac{l_2}{l_1}$ and $\beta = \frac{l_1}{l_2}$.

- Implicit system of equations can be solved using fixed-point iteration, and requires about 5-6 iterations to reach machine precision.

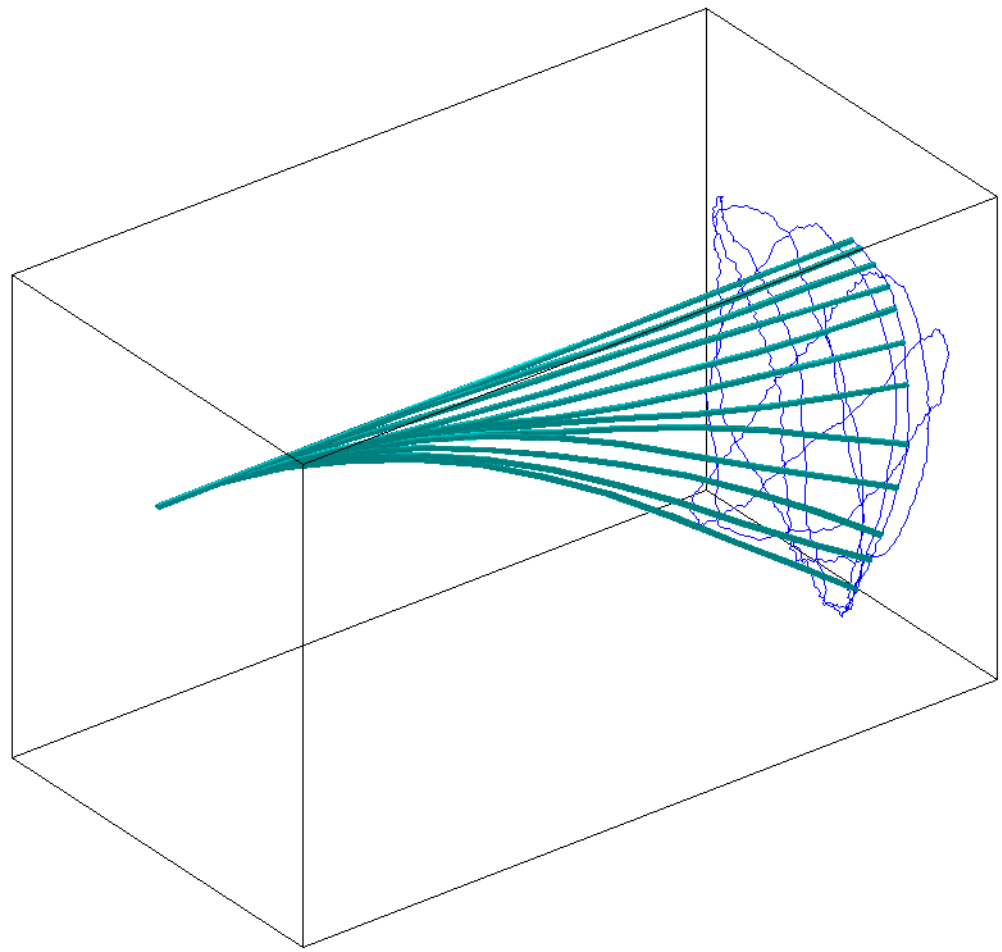
Variational Integrators for S^2

Double Spherical Pendulum Simulation



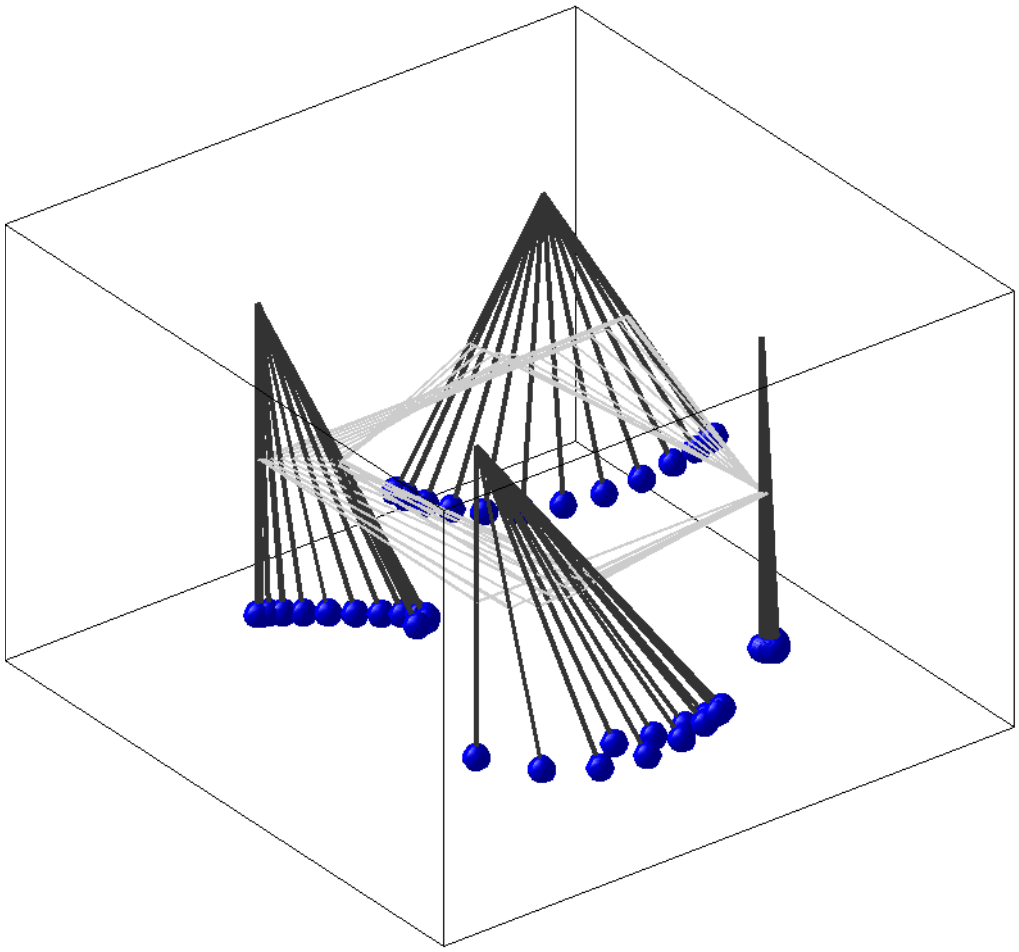
Variational Integrators for S^2

- Elastic Rod



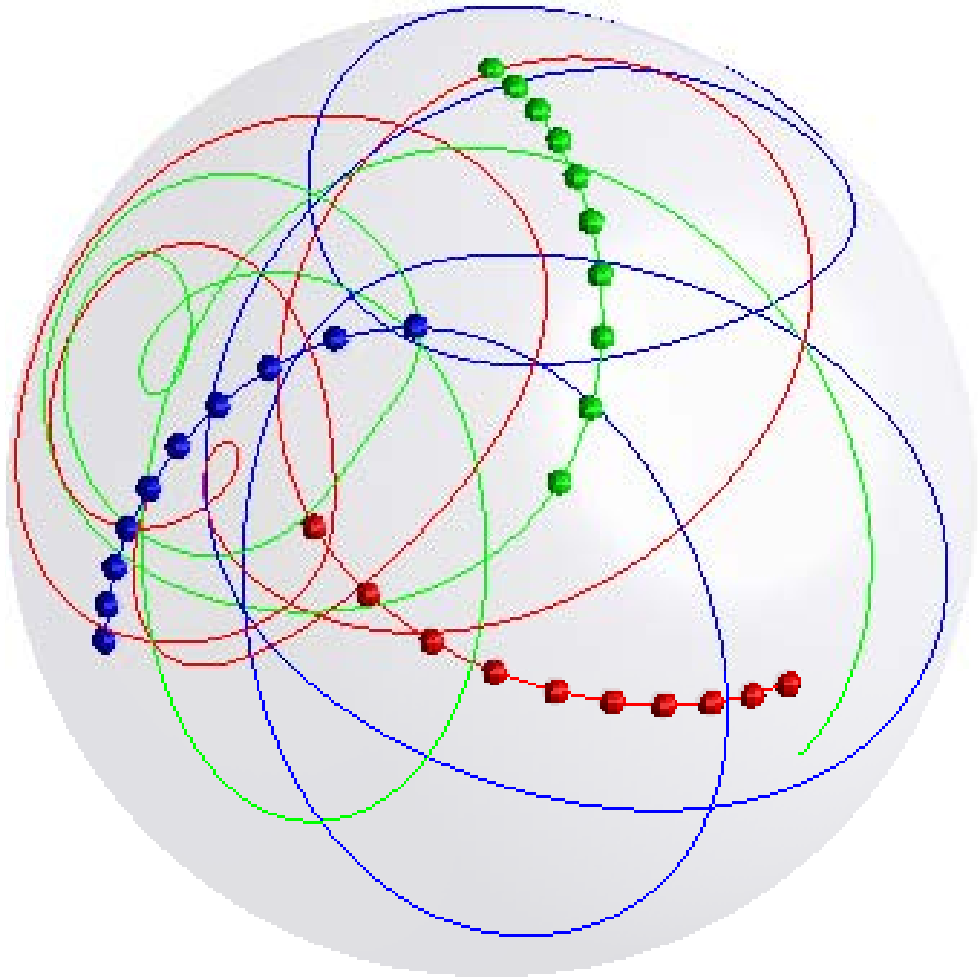
Variational Integrators for S^2

Coupled Spherical Pendula



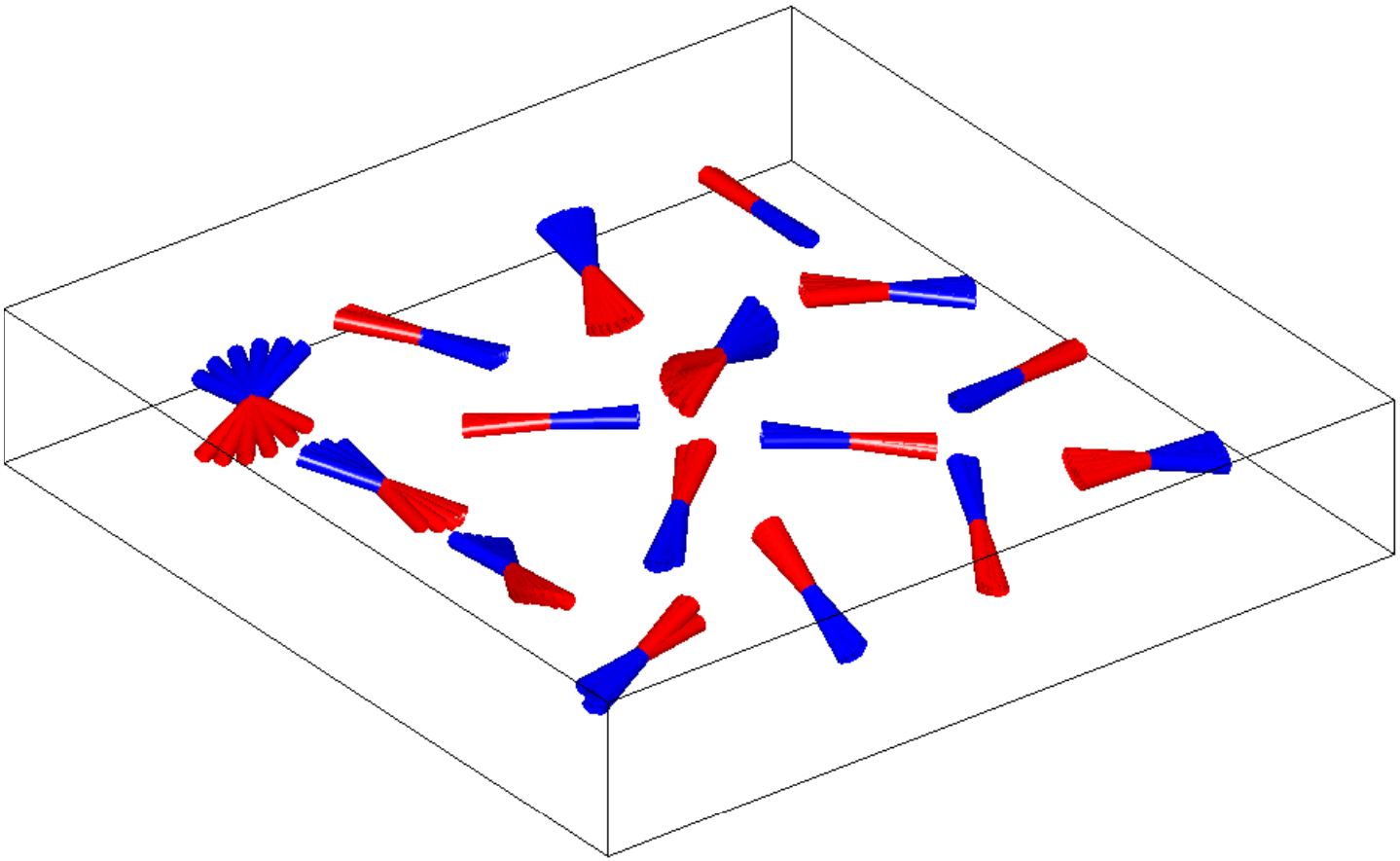
Variational Integrators for S^2

- 3-body problem on the sphere



Variational Integrators for S^2

- Magnetic Arrays



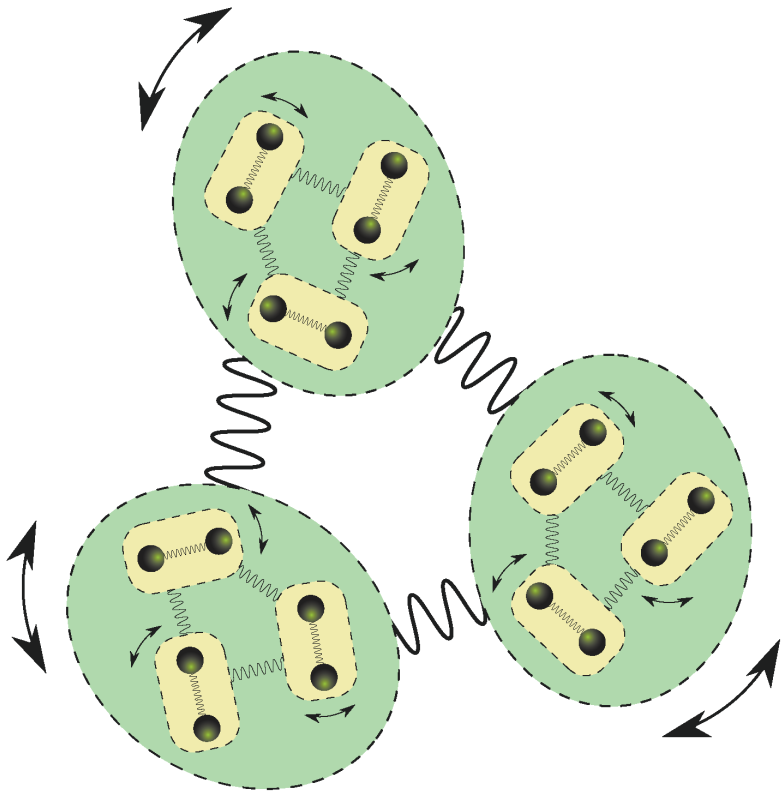
Towards Larger-Scale Scientific Computing Problems

Hierarchical Multi-Resolution Lie Group VIs

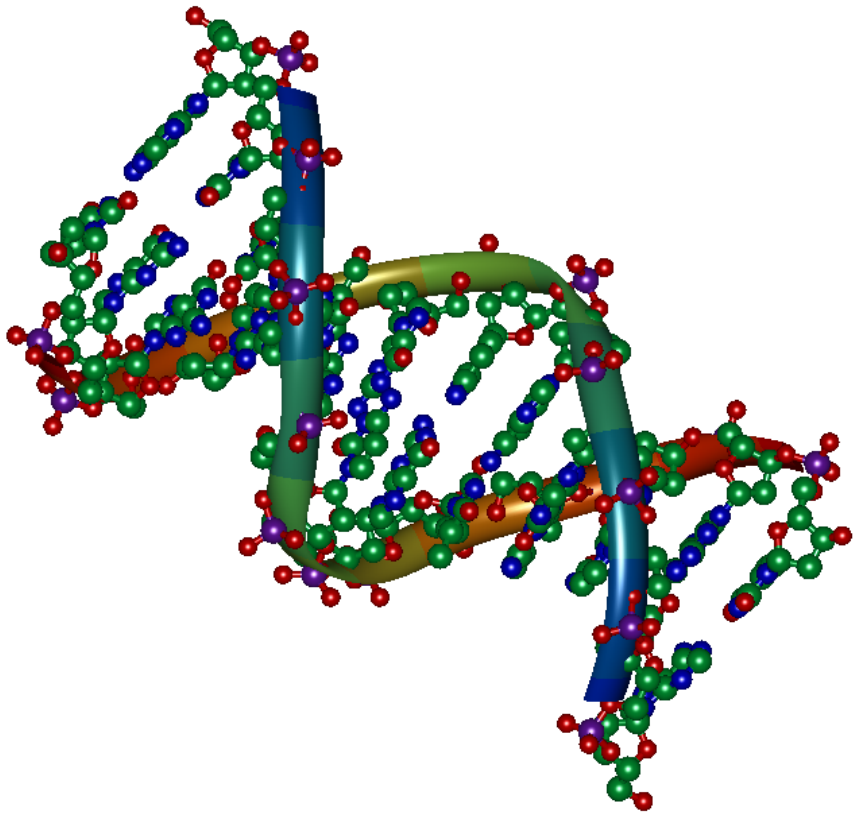
- General framework motivated by multiscale multiphysics methods.
- Based on the use of **empirical shape functions** obtained from localized simulations.
- Decompose a strand of DNA into its constituent nucleotides, and simulate the free nucleotide dynamics to obtain shape functions.
- Incorporate empirical shape functions into larger scale simulation using rigid body deformations of lower level solutions.
- Rigid-body motions form a closed category under recursion.
- Allows for **computational compression** by reusing redundant computations.

Towards Larger-Scale Scientific Computing Problems

Hierarchical Multi-Resolution Lie Group VIs



Schematic of hierarchical method



Strand of DNA composed of nucleotides